

Ground states and dynamics of Bose-Einstein condensation with higher order interactions

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Abstract We analyze the ground states and dynamics of a Bose-Einstein condensate in the presence of a higher order interaction (HOI), modeled by a modified Gross-Pitaevskii equation (MGPE). In fact, due to the appearance of the HOI, the ground state structures become very rich and complicated. We establish the existence and uniqueness as well as non-existence results under different parameter regimes and obtain their limiting behaviors and/or structures under different combinations of HOI and contact interaction strengths. Different structures of ground states are identified for the MGPE with either a harmonic potential or a box potential. Finally, the dynamics of the center-of-mass is investigated and an analytical solution of the MGPE is constructed.

Keywords Bose-Einstein condensation · higher order interaction · Gross-Pitaevskii equation · ground state · dynamics

Mathematics Subject Classification (2000) 35Q55 · 35A01 · 81Q99

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1 Introduction

Bose-Einstein condensation (BEC) has been thoroughly studied since its first experimental realization in 1995 [1, 14] based on the mean-field Gross-Pitaevskii equation (GPE) [31, 6, 2]. In the derivation of the GPE, one key assumption is that the binary interaction between the particles can be well described by the shape-independent approximation (or pseudopotential approximation), i.e. a Dirac function as the interaction kernel, where the interaction strength is characterized by the s -wave scattering length [16]. It is well-known that such an approximation is valid in low energies (or low densities) and becomes less valid in high energies (or high densities) [31, 38, 33]. Therefore, numerous efforts have been devoted to the improvement of the pseudopotential approximation for the two-body interaction, which would lead better mean field theory towards the understanding of recent BEC experiments [38].

Recently, a higher order interaction (HOI) correction to the pseudopotential approximation has been proposed and analyzed [12, 16, 35]. As a consequence, at temperature T much smaller than the critical temperature T_c , a BEC with an HOI can be described by the wave function $\psi := \psi(\mathbf{x}, t)$ whose evolution is governed by the modified Gross-Pitaevskii equation (MGPE) in three dimensions (3D) [12, 16, 35]

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + \tilde{V}(\mathbf{x}) + \tilde{g}_0(|\psi|^2 + \tilde{g}_1\nabla^2|\psi|^2) \right] \psi. \quad (1.1)$$

Here, t is time, $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ is the Cartesian coordinate vector, \hbar is the Planck constant, m is the mass of the particle, $\tilde{g}_0 = \frac{4\pi\hbar^2 a_s}{m}$ is the contact interaction strength with a_s being the s -wave scattering length (positive for repulsive interaction and negative for attractive interaction), $\tilde{g}_1 = \frac{a_s^2}{3} - \frac{a_s r_e}{2}$ is the HOI strength with r_e being the effective range of the two-body interaction and $r_e = \frac{2}{3}a_s$ for hard sphere potential, $\tilde{V}(\mathbf{x})$ is a given real-valued external trapping potential. In typical current experiments, the following harmonic potential is commonly used

$$\tilde{V}(\mathbf{x}) = \frac{m}{2} [\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2], \quad \mathbf{x} = (x, y, z)^T \in \mathbb{R}^3, \quad (1.2)$$

where $\omega_x > 0$, $\omega_y > 0$ and $\omega_z > 0$ are trapping frequencies in x -, y - and z -directions, respectively. The wave function ψ is normalized as

$$\|\psi\|^2 := \int_{\mathbb{R}^3} |\psi(\mathbf{x}, t)|^2 d\mathbf{x} = N, \quad (1.3)$$

where N is the total number of particles in the BEC.

In order to nondimensionalize the MGPE (1.1) with (1.2) and (1.3), we introduce [31, 6, 2]

$$\tilde{t} = \frac{t}{t_s}, \quad \tilde{\mathbf{x}} = \frac{\mathbf{x}}{x_s}, \quad \tilde{\psi}(\tilde{\mathbf{x}}, \tilde{t}) = \frac{x_s^{3/2}}{N^{1/2}} \psi(\mathbf{x}, t), \quad (1.4)$$

where $t_s = \frac{1}{\omega_0}$ and $x_s = \sqrt{\frac{\hbar}{m\omega_0}}$ with $\omega_0 = \min\{\omega_x, \omega_y, \omega_z\}$ are the scaling parameters of dimensionless time and length units, respectively. Plugging (1.4) into (1.1), multiplying by $\frac{t_s^2}{m(x_s N)^{1/2}}$, and then removing all $\tilde{\cdot}$, we obtain the following dimensionless MGPE in 3D for a BEC

$$i\partial_t \psi = \left[-\frac{1}{2} \nabla^2 + V(\mathbf{x}) + g_0 |\psi|^2 - g_1 \nabla^2 |\psi|^2 \right] \psi, \quad (1.5)$$

where $g_0 = \frac{4\pi N a_s}{x_s}$, $g_1 = \frac{4\pi N a_s^2 (3r_e - 2a_s)}{6x_s^3}$, $\gamma_x = \frac{\omega_x}{\omega_0}$, $\gamma_y = \frac{\omega_y}{\omega_0}$ and $\gamma_z = \frac{\omega_z}{\omega_0}$, and the dimensionless trapping potential is given by

$$V(\mathbf{x}) = \frac{1}{2} (\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2), \quad \mathbf{x} \in \mathbb{R}^3. \quad (1.6)$$

When the trapping potential in (1.6) is strongly anisotropic, e.g. $\max\{\gamma_x, \gamma_y\} \ll \gamma_z$ for a quasi-2D BEC or $\gamma_x \ll \min\{\gamma_y, \gamma_z\}$ for a quasi-1D BEC, similar to the dimension reduction of the conventional GPE for BEC [6, 2, 10, 31], the MGPE (1.5) in 3D can be formally reduced to two dimensions (2D) or one dimension (1D) for the disk-shaped or cigar-shaped BEC [38], respectively. In fact, the resulting MGPE can be written in a unified form in d -dimensions ($d = 1, 2, 3$) with $\mathbf{x} \in \mathbb{R}^d$ (denoted as $\mathbf{x} = x \in \mathbb{R}$ for $d = 1$, $\mathbf{x} = (x, y)^T \in \mathbb{R}^2$ for $d = 2$ and $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ for $d = 3$) as

$$i\partial_t \psi = \left[-\frac{1}{2} \nabla^2 + V(\mathbf{x}) + \beta |\psi|^2 - \delta \nabla^2 |\psi|^2 \right] \psi, \quad (1.7)$$

where

$$V(\mathbf{x}) = \begin{cases} \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2), & d = 3, \\ \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2), & d = 2, \\ \frac{1}{2}\gamma_x^2 x^2, & d = 1; \end{cases} \quad (1.8)$$

and β and δ are two dimensionless real constants for describing the contact interaction and HOI strengths, respectively.

For other potentials such as box potential, optical lattice potential and double-well potential, we refer to [6, 31, 4] and references therein. Thus, in the subsequent discussion, we will treat the external potential $V(\mathbf{x})$ in (1.7) as a general real-valued function and the parameters β and δ as arbitrary real constants. In addition, without loss of generality, we assume $V(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^d$ in the rest of this paper. The dimensionless MGPE (1.7) conserves the total mass, i.e.

$$N(t) := \|\psi(\cdot, t)\|^2 = \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 d\mathbf{x} \equiv \|\psi(\cdot, 0)\|^2 = 1, \quad t \geq 0, \quad (1.9)$$

and the energy per particle

$$E(\psi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \psi|^2 + V(\mathbf{x}) |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{\delta}{2} |\nabla |\psi|^2|^2 \right] d\mathbf{x}. \quad (1.10)$$

Theoretically, other higher order terms can be included in the MGPE (1.7) as the higher order corrections of the two-body interaction [12]. Here, we focus on the current MGPE (1.7) to understand the effect of the HOI to the conventional GPE for BEC. In fact, the MGPE (1.7) has been found in other applications (in a generalized form), such as the modelling of ultrashort laser pulses in plasmas [11, 15], the description of the thin-film superfluid condensates [21] and the study of the Heisenberg ferromagnets [36].

The MGPE (1.7) with $\delta = 0$ has been thoroughly studied in the literature and we refer the readers to [6, 2, 31] and references therein. However, there have been only a few mathematical results for the MGPE (1.7), including the local well-posedness of the Cauchy problem [32, 29], existence of solutions to the time independent version of (1.7) [24, 25], the stability of standing waves [13], a spectral method for (1.7) [27], etc. To the best of our knowledge, all the known mathematical results for the MGPE (1.7) are not based on the application in BEC and thus have different setups in the trapping potentials and/or parameter regimes. On the contrary, some physical studies for the MGPE (1.7) have been carried out with the application in BEC, such as the ground state properties [18, 37], the dynamical instabilities [33, 34], etc. Very recently, we have studied the dimension reduction of the MGPE from 3D to lower dimensions [35]. Here, we will present some mathematical results on the ground states and dynamics of the MGPE (1.7) for BEC with HOI.

The paper is organized as follows. In section 2, we establish existence and uniqueness as well as non-existence results of ground states under different parameter regimes. In section 3, we study the asymptotic profiles of ground states in different parameter regimes. In section 4, we derive some dynamical properties of the MGPE. Some conclusions are drawn in section 5.

2 Existence and uniqueness for ground states

Introduce the function space

$$X = \left\{ \phi \in H^1(\mathbb{R}^d) \left| \|\phi\|_X^2 = \|\phi\|^2 + \|\nabla\phi\|^2 + \int_{\mathbb{R}^d} V(\mathbf{x})|\phi(\mathbf{x})|^2 d\mathbf{x} < \infty \right. \right\}.$$

The ground state $\phi_g := \phi_g(\mathbf{x})$ of BEC modelled by the MGPE (1.7) is defined as the minimizer of the energy functional (1.10) under the constraint (1.9), i.e.

$$\phi_g := \arg \min_{\phi \in S} E(\phi), \quad (2.1)$$

where S is defined as

$$S := \{ \phi \in X \mid \|\phi\| = 1, \quad E(\phi) < \infty \}. \quad (2.2)$$

Since S is a nonconvex set, the problem (2.1) is a nonconvex minimization problem. In addition, the ground state ϕ_g is a solution of the following nonlinear eigenvalue problem, i.e. Euler-Lagrange equation of the problem (2.1)

$$\mu\phi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\phi|^2 - \delta\nabla^2|\phi|^2 \right] \phi, \quad (2.3)$$

under the normalization constraint $\phi \in S$, where the corresponding eigenvalue (or chemical potential) $\mu := \mu(\phi)$ can be computed as

$$\mu = E(\phi) + \int_{\mathbb{R}^d} \left(\frac{\beta}{2} |\phi|^4 + \frac{\delta}{2} |\nabla |\phi|^2|^2 \right) d\mathbf{x}. \quad (2.4)$$

The following embedding results hold [6].

Lemma 2.1 *Under the assumption that $V(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^d$ is a confining potential, i.e. $\lim_{R \rightarrow \infty} \text{ess inf}_{|\mathbf{x}| \geq R} V(\mathbf{x}) = +\infty$, we have that the embedding $X \hookrightarrow L^p(\mathbb{R}^d)$ is compact provided that the exponent p satisfies*

$$\begin{cases} p \in [2, 6), & d = 3, \\ p \in [2, \infty), & d = 2, \\ p \in [2, \infty], & d = 1. \end{cases} \quad (2.5)$$

In 2D, i.e. $d = 2$, let C_b be the best constant in the following inequality [39]

$$C_b := \inf_{0 \neq f \in H^1(\mathbb{R}^2)} \frac{\|\nabla f\|_{L^2(\mathbb{R}^2)}^2 \|f\|_{L^2(\mathbb{R}^2)}^2}{\|f\|_{L^4(\mathbb{R}^2)}^4} = \pi \cdot (1.86225 \dots). \quad (2.6)$$

For the existence and uniqueness of the ground states in (2.1), we have

Theorem 2.1 *(Existence and uniqueness) Suppose $V(\mathbf{x}) \geq 0$ satisfying the confining condition, i.e. $\lim_{|\mathbf{x}| \rightarrow \infty} V(\mathbf{x}) = +\infty$, then there exists a minimizer*

$\phi_g \in S$ of (2.1) if one of the following conditions holds

- (i) $\delta > 0$ when $d = 1, 2, 3$ for all $\beta \in \mathbb{R}$;
- (ii) $\delta = 0$ when $d = 1$ for all $\beta \in \mathbb{R}$, when $d = 3$ for $\beta \geq 0$, and when $d = 2$ for $\beta > -C_b$.

Furthermore, $e^{i\theta} \phi_g$ is also a ground state of (2.1) for any $\theta \in [0, 2\pi)$. In particular, the ground state can be chosen as positive and the positive ground state is unique if $\delta \geq 0$ and $\beta \geq 0$. In contrast, there exists no ground state of (2.1) if one of the following holds

- (i') $\delta < 0$;
- (ii') $\delta = 0$ and $\beta < 0$ when $d = 3$; and $\delta = 0$ and $\beta < -C_b$ when $d = 2$.

The results also apply to the bounded connected open domain $\Omega \subset \mathbb{R}^d$ case, i.e. $V(\mathbf{x}) = +\infty$ when $\mathbf{x} \notin \Omega$. In such case, for any $\delta > 0$, there exists $C_\Omega > 0$ (depending on Ω) such that when $\beta \geq -\delta/C_\Omega$, the positive ground state ϕ_g of (2.1) is unique.

Proof The case with $\delta = 0$ is well-known [23, 6] and thus is omitted here.

- (i) In order to prove the existence, we assume $\delta > 0$. By the inequality [22]

$$|\nabla |\phi(\mathbf{x})|| \leq |\nabla \phi(\mathbf{x})|, \quad \text{a.e. } \mathbf{x} \in \mathbb{R}^d, \quad (2.7)$$

we deduce

$$E(\phi) \geq E(|\phi|), \quad (2.8)$$

where equality holds iff $\phi = e^{i\theta}|\phi|$ for some constant $\theta \in [0, 2\pi)$. It suffices to consider the real non-negative minimizers of (2.1). On the other hand, for any $\phi \in S$, denote $\rho = |\phi|^2$, Nash inequality and Young inequality imply that

$$\int_{\mathbb{R}^d} |\phi|^4 d\mathbf{x} \leq \left[C \int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} \right]^{\frac{4}{d+2}} \|\nabla|\phi|^2\|^{\frac{2d}{d+2}} \leq \frac{C}{\varepsilon} + \varepsilon \|\nabla\rho\|^2, \quad \forall \varepsilon > 0.$$

Thus we can conclude that $E(\phi)$ ($\phi \in S$) is bounded from below

$$E(\phi) \geq \int_{\mathbb{R}^d} \left(\frac{1}{2} |\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\delta}{4} |\nabla|\phi|^2|^2 \right) d\mathbf{x} - C.$$

Taking a nonnegative minimizing sequence $\{\phi_n\}_{n=1}^\infty \subset S$, we find the ϕ_n is uniformly bounded in X and there exists $\phi_\infty \in X$ and a subsequence (denote as the original sequence for simplicity) such that

$$\phi_n \rightharpoonup \phi_\infty \quad \text{in } X. \quad (2.9)$$

Lemma 2.1 ensures that $\phi_n \rightarrow \phi_\infty$ in L^p with p given in the lemma. We also have $\nabla|\phi_n|^2 \rightharpoonup \nabla|\phi_\infty|^2$ in L^2 . Hence we know $\phi_\infty \in S$ with ϕ_∞ being nonnegative. Under the condition $\delta > 0$, we get

$$E(\phi_\infty) \leq \liminf_{n \rightarrow \infty} E(\phi_n) = \min_{\phi \in S} E(\phi), \quad (2.10)$$

which shows that ϕ_∞ is a ground state.

For the case $\beta \geq 0$ and $\delta \geq 0$, we can prove the uniqueness of the nonnegative ground state. In order to do so, denote $\rho = |\phi|^2$, then for $\phi = \sqrt{\rho} \in S$, the energy is

$$E(\sqrt{\rho}) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla\sqrt{\rho}|^2 + V(\mathbf{x})\rho + \frac{\beta}{2}\rho^2 + \frac{\delta}{2} |\nabla\rho|^2 \right] d\mathbf{x}. \quad (2.11)$$

The sum of first three terms in the energy $E(\sqrt{\rho})$ is strictly convex in ρ [23, 6], and the last term is also convex because it is quadratic in ρ and $\delta \geq 0$. Hence, we know $E(\sqrt{\rho})$ is strictly convex in ρ and the uniqueness of the nonnegative ground state follows [23, 6]. In addition, from regularity results (see details in Theorem 2.2 below) and maximal principle [23, 22], we can deduce that the nonnegative ground state is strictly positive.

(ii) We prove the nonexistence when $\delta < 0$. Choosing a non-negative smooth function $\varphi(\mathbf{x}) \in S$ with compact support and denoting $\varphi_\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \varphi(\mathbf{x}/\varepsilon) \in S$, we have

$$E(\varphi_\varepsilon) = \int_{\mathbb{R}^d} \left[\frac{1}{2\varepsilon^2} |\nabla\varphi|^2 + V(\varepsilon\mathbf{x})|\varphi|^2 + \frac{\beta}{2\varepsilon^d} |\varphi|^4 + \frac{\delta}{2\varepsilon^{2+d}} |\nabla|\varphi|^2|^2 \right] d\mathbf{x}. \quad (2.12)$$

From the above equation, we see that $\lim_{\varepsilon \rightarrow 0^+} E(\varphi_\varepsilon) \rightarrow -\infty$ if $\delta < 0$ and thus there exists no ground state.

(iii) In the case with $V(\mathbf{x}) = +\infty$ for $\mathbf{x} \notin \Omega$, we know $\phi_g \in H_0^1(\Omega)$. Using Sobolev inequality, there exists $C_\Omega > 0$ such that

$$\|f\|_{L^2(\Omega)} \leq C_\Omega \|\nabla f\|_{L^2(\Omega)}, \quad \forall f \in H_0^1(\Omega). \quad (2.13)$$

Denote $\rho = |\phi|^2$, then for $\phi = \sqrt{\rho} \in S$, we claim the energy $E(\sqrt{\rho})$ is convex in ρ for $\beta \geq -\delta/C_\Omega$. To see this, we only need examine the case $\beta \in [-\delta/C_\Omega, 0)$. For any $\sqrt{\rho_j} \in S$ ($j = 1, 2$) with $\rho_j \in H_0^1(\Omega)$ and $\theta \in [0, 1]$, we have

$$\begin{aligned} & \theta E(\sqrt{\rho_1}) + (1 - \theta)E(\sqrt{\rho_2}) - E(\sqrt{\theta\rho_1 + (1 - \theta)\rho_2}) \\ & \geq \frac{1}{2}\theta(1 - \theta) (\beta\|\rho_1 - \rho_2\|^2 + \delta\|\nabla(\rho_1 - \rho_2)\|^2) \\ & \geq \frac{1}{2}\theta(1 - \theta) (-\delta\|\nabla(\rho_1 - \rho_2)\|^2 + \delta\|\nabla(\rho_1 - \rho_2)\|^2) = 0, \end{aligned}$$

where we used the fact $\|\nabla\sqrt{\rho}\|^2$ is convex in ρ . This shows $E(\sqrt{\rho})$ is convex when $\beta \geq -\frac{\delta}{C_\Omega}$. The uniqueness follows. In the general whole space case, the energy functional $E(\sqrt{\rho})$ is no longer convex and the uniqueness when $\beta < 0$ is in general not clear. We remark here that some recent results were obtained by Guo et al. in [19] about the uniqueness when $\delta = 0$ with $\beta < 0$ and $|\beta|$ is small. \square

Concerning the ground state of (2.1), we have the following properties.

Theorem 2.2 *Let $\delta > 0$ and $\phi_g \in S$ be the nonnegative ground state of (2.1), we have the following properties:*

- (i) *There exists $\alpha > 0$ and $C > 0$ such that $|\phi_g(\mathbf{x})| \leq Ce^{-\alpha|\mathbf{x}|}$ for $\mathbf{x} \in \mathbb{R}^d$.*
- (ii) *If $V(\mathbf{x}) \in L_{\text{loc}}^\infty(\mathbb{R}^d)$, we have ϕ_g is once continuously differentiable and $\nabla\phi_g$ is Hölder continuous with order 1. In particular, if $V(\mathbf{x}) \in C^\infty$, ϕ_g is smooth.*

Proof (i) We show the L^∞ bound of ϕ_g by a Moser's iteration and De Giorgi's iteration following [25]. From the fact that $\phi_g \in S$ minimizes the energy (1.10), it is easy to check that ϕ_g satisfies the Euler-Lagrange equation (2.3), which shows that for any test function $\varphi \in C_0^\infty(\mathbb{R}^d)$, the following holds for $\phi = \phi_g$ and $\mu = \mu(\phi_g)$

$$\int_{\mathbb{R}^d} \left[\frac{1}{2} \nabla\phi \cdot \nabla\varphi + V(\mathbf{x})\phi\varphi + 2\delta\phi\nabla\phi \cdot \nabla(\phi\varphi) \right] d\mathbf{x} = \int_{\mathbb{R}^d} [-\beta|\phi|^2\phi\varphi + \mu\phi\varphi] d\mathbf{x}. \quad (2.14)$$

Using the Moser and De Giorgi iterations, we will prove that any weak solution $\phi \in X \cap \{E(\phi) < \infty\}$ of (2.14) is bounded and decays exponentially as $|\mathbf{x}| \rightarrow \infty$. In detail, we first observe that by an approximation argument, the test function φ can be any functions in X such that $\int_{\mathbb{R}^d} |\varphi|^2 |\nabla\phi|^2 d\mathbf{x} < \infty$ and $\int_{\mathbb{R}^d} |\phi|^2 |\nabla\varphi|^2 d\mathbf{x} < \infty$.

Firstly, we show that for all $q \geq 1$, $\int_{\mathbb{R}^d} (1 + \phi^{2q}) |\nabla\phi|^2 d\mathbf{x} < \infty$. Choosing $q_0 = 12$, since $\nabla\phi^2 \in L^2$ and $\phi \in H^1$, we can get that $\phi \in L^p(\mathbb{R}^d)$ for $p \in [2, q_0]$

and $d = 1, 2, 3$. Let $M > 0$ and

$$\phi_M(\mathbf{x}) = \begin{cases} M, & \phi(\mathbf{x}) > M, \\ \phi(\mathbf{x}), & |\phi(\mathbf{x})| \leq M, \\ -M, & \phi(\mathbf{x}) < -M, \end{cases} \quad \mathbf{x} \in \mathbb{R}^d,$$

and take $\varphi = |\phi_M|^{q_0-4}\phi_M$ as the test function. Plugging $\varphi = |\phi_M|^{q_0-4}\phi_M$ into (2.14), we obtain

$$\begin{aligned} (q_0 - 3) \int_{\mathbb{R}^d} \left(\frac{1}{2} + 2\delta\phi^2 \right) |\phi_M|^{q_0-4} \nabla \phi \cdot \nabla \phi_M d\mathbf{x} + 2\delta \int_{\mathbb{R}^d} \phi \phi_M |\phi_M|^{q_0-4} |\nabla \phi|^2 d\mathbf{x} \\ + \int_{\mathbb{R}^d} V(\mathbf{x}) \phi \phi_M |\phi_M|^{q_0-4} d\mathbf{x} = \int_{\mathbb{R}^d} (-\beta|\phi|^2\phi + \mu\phi) |\phi_M|^{q_0-4} \phi_M d\mathbf{x}. \end{aligned}$$

Letting $M \rightarrow \infty$, we get

$$2(q_0 - 2)\delta \int_{\mathbb{R}^d} |\phi|^{2\tilde{q}} |\nabla \phi|^2 d\mathbf{x} + \int_{\mathbb{R}^d} V(\mathbf{x}) |\phi|^{2\tilde{q}} d\mathbf{x} \leq \int_{\mathbb{R}^d} (|\beta||\phi|^{q_0} + |\mu||\phi|^{q_0-2}) d\mathbf{x}, \quad (2.15)$$

which shows $\int_{\mathbb{R}^d} |\phi|^{\tilde{q}} |\nabla \phi|^2 d\mathbf{x} < \infty$ with $\tilde{q} = \frac{q_0}{2} - 1$. So $\nabla \phi^{\tilde{q}+1} \in L^2$ and for $q_1 = 6\tilde{q} = 3q_0 = 36$, $\phi \in L^p(\mathbb{R}^d)$ for $p \in [2, q_1]$ and $d = 1, 2, 3$. Then, the Moser iteration can continue with $q_j = 3^j q_0$, and $\phi \in L^{q_j}(\mathbb{R}^d)$ (it is obvious when $d = 1, 2$) which verifies our claim. In particular $\phi \in L^p$ for any $p \in [2, \infty)$.

Secondly, we show that $\phi \in L^\infty(\mathbb{R}^d)$ and $\lim_{|\mathbf{x}| \rightarrow \infty} \phi(\mathbf{x}) = 0$ by De Giorgi's iteration. Denoting $f = -\beta|\phi|^2\phi + \mu\phi$ and choosing the test function $\varphi(\mathbf{x}) = (\xi(\mathbf{x}))^2(\phi(\mathbf{x}) - k)_+$ with $k \geq 0$ in (2.14), where $(g(\mathbf{x}))_+ = \max\{g(\mathbf{x}), 0\}$ and $\xi(\mathbf{x})$ is a smooth cutoff function, we have

$$\begin{aligned} \int_{\mathbb{R}^d} \left[\left(\frac{1}{2} + 2\delta\phi^2 + 2\delta\phi(\phi - k)_+ \right) |\xi|^2 |\nabla(\phi - k)_+|^2 + V(\mathbf{x}) |\xi|^2 \phi(\phi - k)_+ \right] d\mathbf{x} \\ = \int_{\mathbb{R}^d} [-(1 + 4\delta\phi^2)(\phi - k)_+ \xi \nabla(\phi - k)_+ \cdot \nabla \xi + f \xi^2 (\phi - k)_+] d\mathbf{x}. \end{aligned}$$

Cauchy inequality gives that

$$\begin{aligned} \int_{\mathbb{R}^d} -(1 + 4\delta\phi^2)(\phi - k)_+ \xi \nabla(\phi - k)_+ \cdot \nabla \xi d\mathbf{x} \\ \leq \varepsilon \int_{\mathbb{R}^d} (1 + \phi^2) |\nabla(\phi - k)_+|^2 d\mathbf{x} + C_\varepsilon \int_{\mathbb{R}^d} (1 + \phi^2) |\nabla \xi|^2 (\phi - k)_+^2 d\mathbf{x}. \end{aligned}$$

Now choosing sufficiently small $\varepsilon > 0$ and defining the function $\Phi_k(\mathbf{x}) = (1 + \phi)(\phi - k)_+$, we can get

$$\int_{\mathbb{R}^d} |\nabla \Phi_k|^2 |\xi|^2 d\mathbf{x} \leq C \int_{\mathbb{R}^d} |\nabla \xi|^2 \Phi_k^2 d\mathbf{x} + C \int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 d\mathbf{x}, \quad (2.16)$$

and

$$\int_{\mathbb{R}^d} |\nabla(\xi \Phi_k)|^2 d\mathbf{x} \leq C \int_{\mathbb{R}^d} |\nabla \xi|^2 \Phi_k^2 d\mathbf{x} + C \int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 d\mathbf{x}. \quad (2.17)$$

Since $f = -\beta|\phi|^2\phi + \mu\phi \in L^q(\mathbb{R}^d)$ for any $2 \leq q < \infty$, we can proceed to obtain L^∞ bound of ϕ by De Giorgi's iteration. Let $B_r(\mathbf{x})$ be the ball centered at \mathbf{x} with radius $r > 0$, and we use B_r for short to denote the ball centered at the origin. For $0 < r < R \leq 1$, we choose C_0^∞ nonnegative cutoff function $\xi(\mathbf{x}) = 1$ for $\mathbf{x} \in B_r(\mathbf{x}_0)$ and $\xi(\mathbf{x}) = 0$ for $\mathbf{x} \notin B_R(\mathbf{x}_0)$ such that $|\nabla \xi(\mathbf{x})| \leq \frac{2}{R-r}$. Since for large q ,

$$\int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 d\mathbf{x} \leq \|\xi f\|_{L^q} \|(\phi - k)_+ \xi\|_{L^6} |\{\Phi_k \xi > 0\}|^{\frac{5}{6} - \frac{1}{q}}, \quad (2.18)$$

where $|A|$ denotes the Lebesgue measure of the set A , for any $\varepsilon > 0$, we have by Hölder inequality and Sobolev inequality in 2D and 3D

$$\begin{aligned} & \int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 d\mathbf{x} \\ & \leq C \|\xi f\|_{L^q} \|\nabla((\phi - k)_+ \xi)\| |\{\Phi_k \xi > 0\}|^{\frac{5}{6} - \frac{1}{q}} \\ & \leq \varepsilon \|\nabla((\phi - k)_+ \xi)\|^2 + C_\varepsilon \|\xi f\|_{L^q}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3} - \frac{2}{q}} \\ & \leq 4\varepsilon (\|\nabla(\Phi_k \xi)\|^2 + 2\|\Phi_k \nabla \xi\|^2) + C_\varepsilon \|\xi f\|_{L^q}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3} - \frac{2}{q}}. \end{aligned}$$

Thus, from the above inequality and (2.17), we arrive at

$$\|\nabla(\xi \Phi_k)\|^2 \leq C \left(\|\Phi_k \nabla \xi\|^2 + \|\xi f\|_{L^q}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3} - \frac{2}{q}} \right). \quad (2.19)$$

Since $\xi \Phi_k \in H_0^1(B_1(\mathbf{x}_0))$, we conclude by Sobolev inequality that,

$$\|\xi \Phi_k\|^2 \leq \|\xi \Phi_k\|_{L^6}^2 |\{\Phi_k \xi > 0\}|^{1 - \frac{2}{3}} \leq C(d) \|\nabla(\xi \Phi_k)\|^2 |\{\Phi_k \xi > 0\}|^{\frac{2}{3}}. \quad (2.20)$$

By choosing $q = 3$, (2.19) and (2.20) imply that

$$\|\xi \Phi_k\|^2 \leq C \left(\|\Phi_k \nabla \xi\|^2 |\{\Phi_k \xi > 0\}|^{\frac{2}{3}} + \|f\|_{L^3(B_1(\mathbf{x}_0))}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3}} \right). \quad (2.21)$$

Denote

$$A(k, r) = \{\mathbf{x} | \mathbf{x} \in B_r(\mathbf{x}_0), \quad \phi(\mathbf{x}) > k\}. \quad (2.22)$$

For $k > 0$ and $0 < r < R \leq 1$, we have

$$\int_{A(k, r)} \Phi_k^2 d\mathbf{x} \leq C \left[\frac{|A(k, R)|^{\frac{2}{3}}}{(R - r)^2} \int_{A(k, R)} \Phi_k^2 d\mathbf{x} + |A(k, R)|^{\frac{5}{3}} \|f\|_{L^3(B_1(\mathbf{x}_0))}^2 \right]. \quad (2.23)$$

We claim that there exists $\tilde{C} > 0$, such that for $k = \tilde{C} \left[\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|(1 + \phi)\phi\|_{L^2(B_1(\mathbf{x}_0))} \right]$,

$$\int_{A(k, \frac{1}{2})} \Phi_k^2 d\mathbf{x} = 0. \quad (2.24)$$

Taking $h > k > k_0$ and $0 < r < 1$, we find $A(h, r) \subset A(k, r)$ with

$$\int_{A(h, r)} \Phi_h^2 d\mathbf{x} \leq \int_{A(k, r)} \Phi_k^2 d\mathbf{x}. \quad (2.25)$$

In addition, since $\Phi_k = (1 + \phi)(\phi - k)_+$, we have

$$|A(h, r)| = |B_r(\mathbf{x}_0) \cap \{\phi - k \geq h - k\}| \leq \frac{1}{(h - k)^2} \int_{A(k, r)} \Phi_k^2 d\mathbf{x}. \quad (2.26)$$

Choosing $\frac{1}{2} \leq r < R \leq 1$, from (2.23), we get

$$\begin{aligned} & \int_{A(h, r)} \Phi_h^2 d\mathbf{x} \\ & \leq C \left(\frac{1}{(R - r)^2} \int_{A(h, R)} \Phi_h^2 d\mathbf{x} + \|f\|_{L^3(B_1(\mathbf{x}_0))}^2 |A(h, R)| \right) |A(h, R)|^{\frac{2}{3}} \\ & \leq \frac{C}{(h - k)^{\frac{4}{3}}} \left(\frac{1}{(R - r)^2} + \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))}^2}{(h - k)^2} \right) \left(\int_{A(k, R)} \Phi_k^2 d\mathbf{x} \right)^{\frac{5}{3}}, \end{aligned}$$

and

$$\|\Phi_h\|_{L^2(B_r(\mathbf{x}_0))} \leq \frac{C}{(h - k)^{\frac{2}{3}}} \left(\frac{1}{R - r} + \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))}}{h - k} \right) \|\Phi_k\|_{L^2(B_R(\mathbf{x}_0))}^{\frac{5}{3}}. \quad (2.27)$$

Denote the function

$$\chi(k, r) = \|\Phi_k\|_{L^2(B_r(\mathbf{x}_0))}. \quad (2.28)$$

For some value of $k > 0$ to be determined later, we define

$$k_l = \left(1 - \frac{1}{2^l}\right) k, \quad r_l = \frac{1}{2} + \frac{1}{2^{l+1}}, \quad l = 0, 1, 2, \dots, \quad (2.29)$$

then $k_l - k_{l-1} = \frac{k}{2^l}$ and $r_{l-1} - r_l = \frac{1}{2^{l+1}}$. From (2.27), we find

$$\begin{aligned} \chi(k_l, r_l) & \leq C \left(2^{l+1} + \frac{2^l \|f\|_{L^3(B_1(\mathbf{x}_0))}}{k} \right) \frac{2^{\frac{2l}{3}}}{k^{\frac{2}{3}}} (\chi(k_{l-1}, r_{l-1}))^{\frac{5}{3}} \\ & \leq 2C \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))} + k}{k^{\frac{5}{3}}} 2^{\frac{5l}{3}} (\chi(k_{l-1}, r_{l-1}))^{\frac{5}{3}}. \end{aligned}$$

Then, we prove that there exists $\gamma > 1$ such that

$$\chi(k_l, r_l) \leq \frac{\chi(k_0, r_0)}{\gamma^l}, \quad l = 0, 1, 2, \dots \quad (2.30)$$

We will argue by induction. When $l = 0$, it is obvious true. Suppose (2.30) is true for $l - 1$ with $l \geq 1$, i.e.

$$\chi(k_{l-1}, r_{l-1}) \leq \frac{\chi(k_0, r_0)}{\gamma^{l-1}} \Rightarrow (\chi(k_{l-1}, r_{l-1}))^{\frac{5}{3}} \leq \frac{\gamma^{\frac{5}{3}} (\chi(k_0, r_0))^{\frac{2}{3}}}{\gamma^{\frac{2l}{3}}} \cdot \frac{\chi(k_0, r_0)}{\gamma^l}.$$

Then, we have

$$\begin{aligned}\chi(k_l, r_l) &\leq 2C \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))} + k}{k^{\frac{5}{3}}} 2^{\frac{5l}{3}} (\chi(k_l, r_l))^{\frac{5}{3}} \\ &\leq 2C \gamma^{\frac{5}{3}} (\chi(k_0, r_0))^{\frac{2}{3}} \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))} + k}{k^{\frac{5}{3}}} \cdot \frac{2^{\frac{5l}{3}}}{\gamma^{\frac{2l}{3}}} \cdot \frac{\chi(k_0, r_0)}{\gamma^l}.\end{aligned}$$

Let us choose $\gamma > 1$ such that $\gamma^{\frac{2}{3}} = 2^{\frac{5}{3}}$. Now we want to pick k sufficiently large such that

$$2C \gamma^{\frac{5}{3}} \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))} + k}{k} \left(\frac{\chi(k_0, r_0)}{k} \right)^{\frac{2}{3}} \leq 1. \quad (2.31)$$

Choosing $k = \tilde{C}(\|f\|_{L^3(B_1(\mathbf{x}_0))} + \chi(k_0, r_0))$ for sufficiently large \tilde{C} , we get the desired inequality (2.31). This gives that (2.30) is true for l and hence the induction is done. Letting $l \rightarrow \infty$ in (2.30), we find $\chi(k, \frac{1}{2}) = 0$, which implies that

$$\Phi_k(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in B_{\frac{1}{2}}(\mathbf{x}_0), \quad (2.32)$$

i.e.,

$$\begin{aligned}\sup_{B_{\frac{1}{2}}(\mathbf{x}_0)} \phi_+ &\leq \tilde{C} [\|f\|_{L^3(B_1(\mathbf{x}_0))} + \chi(k_0, r_0)] \\ &\leq \tilde{C} [\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|\Phi_0\|_{L^2(B_1(\mathbf{x}_0))}] \\ &\leq \tilde{C} [\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|\phi\|_{L^2(B_1(\mathbf{x}_0))} + \|\phi\|_{L^4(B_1(\mathbf{x}_0))}].\end{aligned}$$

The same estimates applies for $-\phi$ and we can conclude that

$$\|\phi\|_{L^\infty(B_{\frac{1}{2}}(\mathbf{x}_0))} \leq \tilde{C} [\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|\phi\|_{L^2(B_1(\mathbf{x}_0))} + \|\phi\|_{L^4(B_1(\mathbf{x}_0))}].$$

This shows ϕ is bounded and $\lim_{|\mathbf{x}| \rightarrow 0} \phi(\mathbf{x}) = 0$.

Thirdly, we prove that $\int_{\mathbb{R}^d \setminus B_R} (|\nabla \phi|^2 + |\phi|^2) d\mathbf{x}$ decays exponentially as $R \rightarrow \infty$. Choose the test function $\varphi = \eta^2(\mathbf{x})\phi$ in (2.14) with $\eta(\mathbf{x})$ being a smooth nonnegative cutoff function such that $\eta(\mathbf{x}) = 0$ for $\mathbf{x} \in B_R$ and $\eta(\mathbf{x}) = 1$ for $\mathbf{x} \in \mathbb{R}^d \setminus B_{R+1}$, then the following holds

$$\begin{aligned}&\int_{\mathbb{R}^d \setminus B_R} \left[\left(\frac{1}{2} + 4\delta\phi^2 \right) |\nabla \phi|^2 \eta^2 + V(\mathbf{x}) |\phi|^2 \eta^2 + \beta\phi^4 \eta^2 - \mu\phi^2 \eta^2 \right] d\mathbf{x} \\ &= - \int_{B_{R+1} \setminus B_R} (1 + 4\delta\phi^2) \eta \phi \nabla \phi \cdot \nabla \eta d\mathbf{x}.\end{aligned}$$

Since $\lim_{|\mathbf{x}| \rightarrow \infty} V(\mathbf{x}) = \infty$ and ϕ is bounded, we find that for large R ,

$$\int_{\mathbb{R}^d \setminus B_R} (|\phi|^2 + |\nabla \phi|^2) d\mathbf{x} \leq C \int_{B_{R+1} \setminus B_R} (|\phi|^2 + |\nabla \phi|^2) d\mathbf{x}. \quad (2.33)$$

Let $a_n = \int_{\mathbb{R}^d \setminus B_{R_n}} (|\phi|^2 + |\nabla \phi|^2) d\mathbf{x}$ with $R_n = R + n$ ($n = 0, 1, 2, \dots$), then $a_n \leq C(a_{n+1} - a_n)$ and $a_{n+1} \leq \alpha a_n$ with $\alpha = \frac{C}{1+C}$. Hence $a_{n+1} \leq \alpha^n a_0$ which would imply the exponential decay of a_n as well as $\int_{\mathbb{R}^d \setminus B_R} (|\nabla \phi|^2 + |\phi|^2) d\mathbf{x}$.

Lastly, combining the exponential decay of $\int_{\mathbb{R}^d \setminus B_R} (|\nabla \phi|^2 + |\phi|^2) d\mathbf{x}$ and De Giorgi's iteration shown above, we can derive the exponential fall-off of $\phi(\mathbf{x})$.

(ii) The regularity of the ground state ϕ_g can be proved by a change of variable method [24, 13]. Let $v = F(t)$ be the solution to the ODE $F'(t) = \sqrt{\frac{1}{2} + \frac{\delta}{2}t^2}$ with $F(0) = 0$, then $F(t)$ is strictly increasing, and its inverse exists (denoted as $t = G(v)$). Let $u = F(\phi)$, then $\phi = G(u)$ and the energy functional $E(\cdot)$ in (1.10) becomes

$$E(\phi) = \int_{\mathbb{R}^d} \left(|\nabla u|^2 + V(\mathbf{x})G^2(u) + \frac{\beta}{2}G^4(u) \right) d\mathbf{x} := \hat{E}(u). \quad (2.34)$$

$u_g = F(\phi_g)$ is the minimizer of $\hat{E}(u)$ under constraint $\int_{\mathbb{R}^d} G(u)^2 d\mathbf{x} = 1$. It follows that u_g satisfies the following Euler-Lagrange equation (for C_0^∞ test function)

$$-\nabla^2 u + V(\mathbf{x})G(u)G'(u) + \beta|G(u)|^2 G(u)G'(u) = \lambda G(u)G'(u). \quad (2.35)$$

Since ϕ_g is bounded, we know u_g is bounded, hence $G(u_g)$ and $G'(u_g)$ are bounded with $\nabla^2 u_g \in L_{\text{loc}}^\infty$. We conclude that u_g is once continuously differentiable and ∇u_g is Hölder continuous with exponent 1. Noticing that $\nabla^2 \phi_g = G'(u_g)\nabla^2 u_g + G''(u_g)|\nabla u_g|^2$, we find that ϕ_g is once continuously differentiable and $\nabla \phi_g$ is Hölder continuous with exponent 1. In addition, if $V \in C^\infty$, we can obtain $\phi_g \in C^\infty$ by a bootstrap argument using the L^∞ bound of ϕ_g . \square

3 Limiting behavior of ground states

In this section, we consider the behavior of the ground state (2.1) in different β and δ parameter regimes. Two types of typical potentials will be discussed, including the harmonic potential (whole space) and the box potential (bounded domain). We note that our results are valid for more general confining potentials in d ($d = 1, 2, 3$) dimensions.

3.1 Harmonic potential case

When $V(\mathbf{x})$ is taken as the harmonic potential (1.8), we consider the limiting profile of the ground states (2.1) under different sets of parameters δ and β .

For any $\phi(\mathbf{x}) \in S$, choose $\phi^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \phi(\mathbf{x}/\varepsilon) \in S$, i.e.

$$\phi(\mathbf{x}) = \varepsilon^{d/2} \phi^\varepsilon(\varepsilon \mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad (3.1)$$

we find the energy $E(\cdot)$ in (1.10) can be written as

$$\begin{aligned} E(\phi) &= \int_{\mathbb{R}^d} \left[\frac{\varepsilon^2}{2} |\nabla \phi^\varepsilon|^2 + \frac{1}{\varepsilon^2} V(\mathbf{x}) |\phi^\varepsilon|^2 + \frac{\beta \varepsilon^d}{2} |\phi^\varepsilon|^4 + \frac{\delta \varepsilon^{2+d}}{2} |\nabla |\phi^\varepsilon|^2|^2 \right] d\mathbf{x} \\ &:= \frac{1}{\varepsilon^2} E^\varepsilon(\phi^\varepsilon), \end{aligned} \quad (3.2)$$

where

$$E^\varepsilon(\phi^\varepsilon) = \int_{\mathbb{R}^d} \left[\frac{\varepsilon^4}{2} |\nabla \phi^\varepsilon|^2 + V(\mathbf{x}) |\phi^\varepsilon|^2 + \frac{\beta \varepsilon^{d+2}}{2} |\phi^\varepsilon|^4 + \frac{\delta \varepsilon^{4+d}}{2} |\nabla |\phi^\varepsilon|^2|^2 \right] d\mathbf{x}, \quad (3.3)$$

which indicates that

$$\phi_g = \arg \min_{\phi \in S} E(\phi) \stackrel{\phi_g(\mathbf{x}) = \varepsilon^{d/2} \phi_g^\varepsilon(\mathbf{x}/\varepsilon)}{\iff} \phi_g^\varepsilon = \arg \min_{\phi^\varepsilon \in S} E^\varepsilon(\phi^\varepsilon). \quad (3.4)$$

Now, we give the characterization of the ground state ϕ_g of (2.1) when the two types of interaction strength are very large.

Theorem 3.1 (*Thomas-Fermi (TF) limit when $\beta \rightarrow +\infty$*) Let $V(\mathbf{x})$ ($\mathbf{x} \in \mathbb{R}^d$, $d = 1, 2, 3$) be given in (1.8), $\delta > 0$, $\phi_g \in S$ be the positive ground state of (2.1).

(1) If $\beta \rightarrow +\infty$ and $\delta = o(\beta^{\frac{4+d}{2+d}})$, set $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \phi_g(\mathbf{x}/\varepsilon) \in S$ with $\varepsilon = \beta^{-\frac{1}{2+d}}$. For $\beta \rightarrow +\infty$ ($\varepsilon \rightarrow 0^+$), we have $\rho_g^\varepsilon = |\phi_g^\varepsilon(\mathbf{x})|^2$ converges to $\rho_\infty(\mathbf{x}) := |\phi_\infty(\mathbf{x})|^2$ in L^2 , where $\phi_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy

$$E_1(\phi) = \int_{\mathbb{R}^d} \left(V(\mathbf{x}) |\phi|^2 + \frac{1}{2} |\phi|^4 \right) d\mathbf{x} \quad \text{with} \quad \|\phi\| = 1. \quad (3.5)$$

More precisely, $\rho_\infty = |\phi_\infty|^2 = (\mu - V(\mathbf{x}))_+$ with $\mu = E_1(\phi_\infty) + \frac{1}{2} \|\phi_\infty\|_{L^4}^4$.

(2) If $\beta \rightarrow +\infty$ and $\delta = O(\beta^{\frac{4+d}{2+d}})$, i.e. $\lim_{\beta \rightarrow +\infty} \frac{\delta}{\beta^{\frac{4+d}{2+d}}} = \delta_\infty > 0$, set $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \phi_g(\mathbf{x}/\varepsilon) \in S$ with $\varepsilon = \beta^{-\frac{1}{2+d}}$. For $\delta \rightarrow +\infty$ ($\varepsilon \rightarrow 0^+$), we have $\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2$ converges to $\rho_\infty(\mathbf{x})$ in H^1 , where $\phi_\infty(\mathbf{x}) = \sqrt{\rho_\infty(\mathbf{x})}$ is the unique nonnegative minimizer of the energy

$$E_2(\phi) = \int_{\mathbb{R}^d} \left(V(\mathbf{x}) |\phi|^2 + \frac{|\phi|^4}{2} + \frac{\delta_\infty}{2} |\nabla |\phi|^2|^2 \right) d\mathbf{x} \quad \text{with} \quad \|\phi\| = 1. \quad (3.6)$$

The existence of the minimizer ρ_∞ to the energy $E_2(\sqrt{\rho})$ is a similar argument to Theorem 2.1 and the minimizer is unique because $E_2(\sqrt{\rho})$ is convex in ρ .

(3) If $\beta \rightarrow +\infty$ and $\delta/\beta^{\frac{4+d}{2+d}} \gg 1$, i.e. $\beta = o(\delta^{\frac{2+d}{4+d}})$ as $\delta \rightarrow +\infty$, set $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \phi_g(\mathbf{x}/\varepsilon) \in S$ with $\varepsilon = \delta^{-\frac{1}{4+d}}$. For $\delta \rightarrow +\infty$ ($\varepsilon \rightarrow 0^+$), we have $\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2$ converges to $\rho_\infty(\mathbf{x})$ in H^1 , where $\phi_\infty(\mathbf{x}) = \sqrt{\rho_\infty(\mathbf{x})}$ is the unique nonnegative minimizer of the energy

$$E_3(\phi) = \int_{\mathbb{R}^d} \left(V(\mathbf{x}) |\phi|^2 + \frac{1}{2} |\nabla |\phi|^2|^2 \right) d\mathbf{x} \quad \text{with} \quad \|\phi\| = 1. \quad (3.7)$$

The existence of the minimizer ρ_∞ to the energy $E_3(\sqrt{\rho})$ is a similar argument to Theorem 2.1 and the minimizer is unique because $E_3(\sqrt{\rho})$ is convex in ρ .

Proof (1) Using (3.3) and choosing $\varepsilon = \beta^{-\frac{1}{d+2}}$, we find $\phi_g^\varepsilon \in S$ minimizes

$$E^\varepsilon(\phi^\varepsilon) = \int_{\mathbb{R}^d} \left[\frac{\varepsilon^4}{2} |\nabla \phi^\varepsilon|^2 + V(\mathbf{x}) |\phi^\varepsilon|^2 + \frac{|\phi^\varepsilon|^4}{2} + \frac{\delta \varepsilon^{4+d}}{2} |\nabla |\phi^\varepsilon|^2|^2 \right] d\mathbf{x}. \quad (3.8)$$

On the other hand, $E_1(\phi)$ has a unique nonnegative minimizer ϕ_∞ and by an approximation argument, we can take any smooth approximations of $\phi_\infty(\mathbf{x})$ in S and find that for any $\eta > 0$ with $\delta = o(\beta^{\frac{d+4}{d+2}})$

$$E_1(\phi_\infty) \leq E^\varepsilon(\phi_g^\varepsilon) \leq E_1(\phi_\infty) + \eta + C(\eta)(\varepsilon^4 + o(1)),$$

which implies

$$\lim_{\varepsilon \rightarrow 0^+} E_1(\phi_g^\varepsilon) = E_1(\phi_\infty). \quad (3.9)$$

Hence we know ϕ_g^ε ($\varepsilon \rightarrow 0^+$) is a minimizing sequence of $E_1(\cdot)$. On the other hand,

$$\begin{aligned} E_1(\phi_g^\varepsilon) - E_1(\phi_\infty) &= \int_{\mathbb{R}^d} \left[(V(\mathbf{x}) + |\phi_\infty|^2)(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2) + \frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 \right] d\mathbf{x} \\ &= \int_{\mathbb{R}^d} \left[\max\{V(\mathbf{x}), \mu\}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2) + \frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 \right] d\mathbf{x} \\ &\geq \int_{\mathbb{R}^d} \left[\mu|\phi_g^\varepsilon|^2 - \mu|\phi_\infty|^2 + \frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 \right] d\mathbf{x} \\ &= \frac{1}{2} \int_{\mathbb{R}^d} (|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 d\mathbf{x}, \end{aligned}$$

and the conclusion follows.

(2) Similar to the case (1), it is easy to show $\lim_{\varepsilon \rightarrow 0^+} E_2(\phi_g^\varepsilon) = E_2(\phi_\infty)$.

Noticing that for any function $0 \leq \sqrt{\rho(\mathbf{x})} \in H^1$ with $\int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} = 1$, we have $E_2(\sqrt{(\rho_\infty + s\rho)/(1+s)})$ ($s \geq 0$) attains minimum at $s = 0$. By direct computation, we find

$$\begin{aligned} \frac{d}{ds} E_2 \left(\sqrt{\frac{\rho_\infty + s\rho}{1+s}} \right) \Big|_{s=0} &= \int_{\mathbb{R}^d} [(V(\mathbf{x}) + \rho_\infty(\mathbf{x}))\rho(\mathbf{x}) + \delta_\infty \nabla \rho_\infty(\mathbf{x}) \cdot \nabla \rho(\mathbf{x})] d\mathbf{x} \\ &\quad - \int_{\mathbb{R}^d} (V(\mathbf{x})\rho_\infty(\mathbf{x}) + \rho_\infty^2(\mathbf{x}) + \delta_\infty |\nabla \rho_\infty(\mathbf{x})|^2) d\mathbf{x} \\ &\geq 0. \end{aligned}$$

A simple calculation shows

$$\begin{aligned} E_2(\phi_g^\varepsilon) - E_2(\phi_\infty) &= \frac{d}{ds} E_2 \left(\sqrt{\frac{\rho_\infty + s\rho^\varepsilon}{1+s}} \right) \Big|_{s=0} \\ &\quad + \int_{\mathbb{R}^d} \left[\frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 + \frac{\delta_\infty}{2} (\nabla |\phi_g^\varepsilon|^2 - \nabla |\phi_\infty|^2)^2 \right] d\mathbf{x} \\ &\geq \int_{\mathbb{R}^d} \left[\frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 + \frac{\delta_\infty}{2} (\nabla |\phi_g^\varepsilon|^2 - \nabla |\phi_\infty|^2)^2 \right] d\mathbf{x}, \end{aligned}$$

which implies $\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2$ converges to $\rho_\infty(\mathbf{x})$ in H^1 .

(3) Using (3.3) and choosing $\varepsilon = \delta^{-\frac{1}{4+d}}$, we find $\phi_g^\varepsilon \in S$ minimizes

$$E^\varepsilon(\phi^\varepsilon) = \int_{\mathbb{R}^d} \left[\frac{\varepsilon^4}{2} |\nabla \phi^\varepsilon|^2 + V(\mathbf{x}) |\phi^\varepsilon|^2 + \frac{\beta \varepsilon^{d+2} |\phi^\varepsilon|^4}{2} + \frac{1}{2} |\nabla |\phi^\varepsilon|^2|^2 \right] d\mathbf{x}. \quad (3.10)$$

Nash inequality and Young inequality imply that for $\rho^\varepsilon = |\phi^\varepsilon|^2$ with $\phi^\varepsilon \in S$,

$$\int_{\mathbb{R}^d} |\rho^\varepsilon(\mathbf{x})|^2 d\mathbf{x} \leq C \|\rho^\varepsilon\|_{L^1}^{4/(d+2)} \|\nabla \rho^\varepsilon\|^{2d/(d+2)} \leq C + \|\nabla \rho^\varepsilon\|^2.$$

Thus, we conclude that for $\beta = o(\delta^{\frac{2+d}{4+d}})$,

$$E^\varepsilon(\phi^\varepsilon) \geq \int_{\mathbb{R}^d} \left(V(\mathbf{x}) |\phi^\varepsilon|^2 + \frac{1}{2} (1 - o(1)) |\nabla |\phi^\varepsilon|^2|^2 \right) d\mathbf{x} - o(1), \quad \phi^\varepsilon \in S. \quad (3.11)$$

For sufficiently small ε , (3.11) gives that for the ground state ϕ_g^ε ,

$$E_3(\phi_g^\varepsilon) \leq C, \quad (3.12)$$

and we obtain

$$E^\varepsilon(\phi_g^\varepsilon) \geq E_3(\phi_g^\varepsilon) - o(1). \quad (3.13)$$

Choosing smooth approximations of ϕ_∞ in S if necessary, we could get for any $\eta > 0$,

$$E^\varepsilon(\phi_g^\varepsilon) \leq E_3(\phi_\infty) + \eta + C(\eta)(\varepsilon^4 + o(1)). \quad (3.14)$$

Combining (3.13), (3.14) and the fact that ϕ_∞ minimizes E_3 under the constraint $\|\phi\| = 1$, we find that

$$\lim_{\varepsilon \rightarrow 0^+} E_3(\phi_g^\varepsilon) = E_3(\phi_\infty). \quad (3.15)$$

On the other hand, $E_3 \left(\sqrt{(\rho_\infty + s\rho_g^\varepsilon)/(1+s)} \right)$ ($s \geq 0$) reach its minimum at $s = 0$, and

$$\begin{aligned} 0 &\leq \frac{d}{ds} E_3 \left(\sqrt{\frac{\rho_\infty + s\rho_g^\varepsilon}{1+s}} \right) \Big|_{s=0} \\ &= \int_{\mathbb{R}^d} (\rho_g^\varepsilon V(\mathbf{x}) + \nabla \rho_g^\varepsilon \cdot \nabla \rho_\infty) d\mathbf{x} - \int_{\mathbb{R}^d} (\rho_\infty V(\mathbf{x}) + \nabla \rho_\infty \cdot \nabla \rho_\infty) d\mathbf{x}. \end{aligned}$$

Therefore

$$\begin{aligned} &E_1(\phi_g^\varepsilon) - E_1(\phi_\infty) \\ &= \int_{\mathbb{R}^d} ((\rho_g^\varepsilon - \rho_\infty)V + \nabla(\rho_g^\varepsilon - \rho_\infty) \cdot \nabla \rho_\infty) d\mathbf{x} + \frac{1}{2} \|\nabla \rho_g^\varepsilon - \nabla \rho_\infty\|^2 \\ &\geq \frac{1}{2} \|\nabla \rho_g^\varepsilon - \nabla \rho_\infty\|^2. \end{aligned}$$

The convergence of ρ_g^ε towards ρ_∞ as $\varepsilon \rightarrow 0^+$ is then a direct consequence. \square

In Theorem 3.1, three types of limiting profiles are obtained and the usual TF density as the minimizer of the energy $E_1(\cdot)$ in (3.5) has a compact support. We would like to show that the minimizers of the energy functionals $E_2(\cdot)$ in (3.6) and $E_3(\cdot)$ in (3.7) are indeed solutions of certain free boundary problems.

Theorem 3.2 *Let $V(\mathbf{x}) \geq 0$ ($\mathbf{x} \in \mathbb{R}^d$, $d = 1, 2, 3$) be given in (1.8), and nonnegative functions $\rho_1(\mathbf{x}) \geq 0$ and $\rho_2(\mathbf{x}) \geq 0$ be the unique minimizers of $E_2(\sqrt{\rho})$ and $E_3(\sqrt{\rho})$ under the constraints $\|\rho\|_{L^1} = 1$ and $\rho \geq 0$, respectively. Then $\rho_1, \rho_2 \in C_{\text{loc}}^{1,\alpha} \subset W_{\text{loc}}^{2,p}$ ($1 < p < \infty$ and $0 < \alpha < 1$) solve the free boundary value problems*

$$-\delta_\infty \Delta \rho_1 + \rho_1 = (\mu_1 - V(\mathbf{x})) \chi_{\{\rho_1 > 0\}}, \quad \text{a.e. } \mathbf{x} \in \mathbb{R}^d, \quad (3.16)$$

$$-\delta_\infty \Delta \rho_2 = (\mu_2 - V(\mathbf{x})) \chi_{\{\rho_2 > 0\}}, \quad \text{a.e. } \mathbf{x} \in \mathbb{R}^d, \quad (3.17)$$

where $\mu_1 = 2E_2(\sqrt{\rho_1}) - \int_{\mathbb{R}^d} V(\mathbf{x}) \rho_1 d\mathbf{x}$ and $\mu_2 = 2E_3(\sqrt{\rho_2}) - \int_{\mathbb{R}^d} V(\mathbf{x}) \rho_2 d\mathbf{x}$. The conditions at the free boundaries are

$$\rho_j|_{\partial\{\rho_j > 0\}} = 0, \quad |\nabla \rho_j|_{\partial\{\rho_j > 0\}} = 0, \quad j = 1, 2. \quad (3.18)$$

If $V(\mathbf{x})$ is radially symmetric and non-decreasing, $\rho_j(\mathbf{x})$ ($j = 1, 2$) are radially symmetric non-increasing and compactly supported.

Proof (i) We verify the two equations (3.16) and (3.17). The arguments are very similar, and we only prove (3.16) for simplicity.

We adapt an approach for the classical obstacle problem in [30]. Since $\rho_1 \geq 0$ minimizes $E_2(\sqrt{\rho})$ under the constraints $\|\rho\|_{L^1} = 1$ and $\rho \geq 0$, in addition $V(\mathbf{x}) \geq 0$, we can conclude that ρ_1 minimizes the following energy

$$\tilde{E}(\rho) = \int_{\mathbb{R}^d} \left(V(\mathbf{x})|\rho| + \frac{\rho^2}{2} + \frac{\delta_\infty}{2} |\nabla \rho|^2 \right) d\mathbf{x} \quad \text{with} \quad \int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} = 1, \quad (3.19)$$

i.e. ρ_1 is still a minimizer if we remove the nonnegative constraint with the price to have a non-smooth $V(\mathbf{x})|\rho|$ term. The reason is that if $\int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} = 1$, we can write $\rho_+(\mathbf{x}) = \max\{\rho(\mathbf{x}), 0\}$ and $\rho_-(\mathbf{x}) = \max\{-\rho(\mathbf{x}), 0\}$, and $\int_{\mathbb{R}^d} \rho_+(\mathbf{x}) \geq 1$. Since all the terms in the energy $\tilde{E}(\rho)$ are positive, we have $\tilde{E}(\rho_+ / \|\rho_+\|_{L^1}) \leq \tilde{E}(\rho_+) \leq \tilde{E}(\rho)$. Thus, the minimizer must be nonnegative and the unique minimizer of (3.19) (by convexity) is ρ_1 .

Now, we would like to derive the equation for ρ_1 . In order to do this, we introduce the following regularization of (3.19). Mollify the step function $\chi_{[0,\infty)}(s)$ ($s \in \mathbb{R}$) to get smooth function $g_\varepsilon(s) \in C^\infty(\mathbb{R})$ ($\varepsilon > 0$) such that $g_\varepsilon(s) = 1$ if $s > 0$, $g_\varepsilon(s) = 0$ if $s \leq -\varepsilon$ and $g'_\varepsilon(s) \geq 0$ for all $s \in \mathbb{R}$. Moreover, $g_\varepsilon(s) \rightarrow \chi_{(0,\infty)}$ as $\varepsilon \rightarrow 0^+$. Denote $G_\varepsilon(s) = \int_{-\infty}^s g_\varepsilon(s) ds$ and $G''_\varepsilon \geq 0$ indicating that G_ε is a convex function. Now, let us consider

$$\tilde{E}^\varepsilon(\rho) = \int_{\mathbb{R}^d} \left(V(\mathbf{x})G_\varepsilon(\rho) + \frac{\rho^2}{2} + \frac{\delta_\infty}{2} |\nabla \rho|^2 \right) d\mathbf{x} \quad \text{with} \quad \int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} = 1, \quad (3.20)$$

which is still a convex minimization problem and we have a unique minimizer $\rho_g^\varepsilon(\mathbf{x})$. Moreover, we can find the equations for $\rho_g^\varepsilon(\mathbf{x})$.

For any compactly supported smooth function $\varphi \in C_c^\infty(\mathbb{R}^d)$, consider $h(s) = \tilde{E}^\varepsilon(\rho_s(\mathbf{x}))$ where $\rho_s(\mathbf{x}) = (\rho_g^\varepsilon + s\varphi) / \int_{\mathbb{R}^d} (\rho_g^\varepsilon + s\varphi) d\mathbf{x}$ and $s \in (-s_0, s_0)$ with sufficiently small $s_0 > 0$ such that $\int_{\mathbb{R}^d} (\rho_g^\varepsilon + s\varphi) d\mathbf{x} \geq 1/2$, we then have $h(s)$ attains its minimum at $s = 0$. By standard computations and arguments [17, 22], we can get that there exists a Lagrange multiplier μ_ε , such that ρ_g^ε solves (in the weak sense)

$$-\delta_\infty \Delta \rho_g^\varepsilon + \rho_g^\varepsilon = \mu_\varepsilon - V(\mathbf{x}) g_\varepsilon(\rho_g^\varepsilon). \quad (3.21)$$

It is easy to see that μ_ε is uniformly bounded and $\mu_\varepsilon - V(\mathbf{x}) g_\varepsilon(\rho_g^\varepsilon) \in L_{\text{loc}}^\infty$, which implies that for any bounded smooth domain $\Omega \subset \mathbb{R}^d$, ρ_g^ε is uniformly bounded in $W^{2,p}(\Omega)$ ($p \in (1, \infty)$) by classical elliptic regularity results [17, 22]. Using Sobolev embedding, ρ_g^ε is uniformly bounded in $C^{1,\alpha}(\Omega)$ (for some $0 < \alpha < 1$) locally and hence there exist $\tilde{\rho} \in W^{2,p}(\Omega)$ such that as $\varepsilon \rightarrow 0^+$ (take a subsequence $\varepsilon_k \rightarrow 0^+$ if necessary), ρ_g^ε converges to $\tilde{\rho}$ strongly in $C_{\text{loc}}^{1,\alpha}$ and weakly in $W_{\text{loc}}^{2,p}$. Consequently, $\int_{\mathbb{R}^d} \tilde{\rho} d\mathbf{x} = 1$ ($V(\mathbf{x})$ is a confining potential). In fact, we can show $\tilde{\rho} = \rho_1$. Passing to the limit as $\varepsilon \rightarrow 0^+$ in $\tilde{E}(\rho_g^\varepsilon) \leq \tilde{E}^\varepsilon(\rho_g^\varepsilon) \leq \tilde{E}^\varepsilon(\rho_1)$ ($G_\varepsilon(|s|) \geq |s|$), we observe that $\tilde{E}(\tilde{\rho}) \leq \limsup_{\varepsilon \rightarrow 0^+} \tilde{E}^\varepsilon(\rho_g^\varepsilon) \leq \tilde{E}(\rho_1)$ and it is obvious $\tilde{\rho} = \rho_1$.

Now, we have $\rho_1 \in W_{\text{loc}}^{2,p} \cap C_{\text{loc}}^{1,\alpha}$ and we want to show that

$$-\delta_\infty \Delta \rho_1 + \rho_1 = (\mu - V(\mathbf{x})) \chi_{\{\rho_1 > 0\}}, \quad \text{a.e. } \mathbf{x} \in \mathbb{R}^d. \quad (3.22)$$

Since $\rho_g^\varepsilon \in W_{\text{loc}}^{2,p}$ is a strong solution of (3.21), thus (3.21) is valid almost everywhere. In addition, $\rho_g^\varepsilon \rightarrow \rho_1$ in $C_{\text{loc}}^{1,\alpha}$, so we can pass to the limit as $\varepsilon \rightarrow 0^+$ in (3.21) to get

$$-\delta_\infty \Delta \rho_1 + \rho_1 = \mu - V(\mathbf{x}), \quad \text{a.e. } \mathbf{x} \in \{\rho_1 > 0\}, \quad (3.23)$$

where μ is a limiting point of μ_ε as $\varepsilon \rightarrow 0^+$ (take a subsequence if necessary here). On the other hand, $\rho_1 \in W_{\text{loc}}^{2,p}$ implies $\Delta \rho_1 = 0$ a.e. $\mathbf{x} \in \{\rho_1 = 0\}$. Together, we have shown ρ_1 is the solution of the free boundary value problem (3.16) and μ can be computed via multiplying both sides of (3.16) by ρ_1 and integrating over \mathbb{R}^d , which leads to $\mu = \mu_1$.

(ii) When $V(\mathbf{x}) = V(r)$ ($r = |\mathbf{x}|$) is radially symmetric and non-decreasing, it is easy to find $\rho_j(\mathbf{x})$ is radially symmetric and non-increasing by Schwarz rearrangement [22]. For simplicity, we write $\rho_j(\mathbf{x}) = \rho_j(|\mathbf{x}|) = \rho_j(r)$ ($r = |\mathbf{x}|$, $j = 1, 2$) and it holds $\rho_j'(r) \leq 0$. Integrating (3.16) over the ball $B_R = \{|\mathbf{x}| < R\}$, we get

$$\int_{B_R} (V(\mathbf{x}) \chi_{\{\rho_1 > 0\}} + \rho_1(\mathbf{x})) d\mathbf{x} - \delta_\infty \int_{\partial B_R} \partial_n \rho_1(\mathbf{x}) dS = \mu_1 \int_{B_R} \chi_{\{\rho_1 > 0\}} d\mathbf{x},$$

where $\partial_{\mathbf{n}}\rho_1(\mathbf{x})|_{\partial B_R} \leq 0$ ($\rho_1(r)$ is non-increasing). On the other hand, $\lim_{r \rightarrow \infty} V(r) = \infty$, choosing R_0 large enough such that $V(r) \geq 2\mu_1$ ($r \geq R_0$), we have

$$\int_{B_R \setminus B_{R_0}} [(V(\mathbf{x}) - \mu_1)\chi_{\{\rho_1 > 0\}} + \rho_1(\mathbf{x})] d\mathbf{x} \leq \mu_1 |B_{R_0}|,$$

which is true for all $R > R_0$. Thus, we arrive at

$$|B_{R_0}^c \cap \chi_{\{\rho_1 > 0\}}| \leq |B_{R_0}|, \quad (3.24)$$

and it implies that $|\{\rho_1 > 0\}| < \infty$. Therefore ρ_1 is compactly supported. Similarly, ρ_2 is also compactly supported under the hypothesis of $V(\mathbf{x})$. \square

Next, we consider another interesting case that $\beta \rightarrow -\infty$ and/or large δ .

Theorem 3.3 (*Limits when $\beta \rightarrow -\infty$*) Let $V(\mathbf{x})$ ($\mathbf{x} \in \mathbb{R}^d$, $d = 1, 2, 3$) be given in (1.8), $\beta < 0$, $\delta > 0$, $\phi_g \in S$ be a nonnegative ground state of (2.1).

(1) If $\beta \rightarrow -\infty$ and $\delta = O(|\beta|^{\frac{4+d}{2+d}})$, i.e. $\lim_{\beta \rightarrow +\infty} \frac{\delta}{|\beta|^{\frac{4+d}{2+d}}} = \delta_\infty > 0$, set $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \phi_g(\mathbf{x}/\varepsilon) \in S$ with $\varepsilon = |\beta|^{-\frac{1}{2+d}}$. For $\beta \rightarrow -\infty$ ($\varepsilon \rightarrow 0^+$), there exists a subsequence $\beta_n \rightarrow -\infty$ ($n = 1, 2, \dots$), such that for $\varepsilon_n = |\beta_n|^{-\frac{1}{2+d}} \rightarrow 0^+$ and $\rho_g^{\varepsilon_n}(\mathbf{x}) = \varepsilon_n^{-d} |\phi_g(\mathbf{x}/\varepsilon_n)|^2$, we have $\rho_g^{\varepsilon_n}(\mathbf{x}) \rightarrow \rho_g(\mathbf{x})$ in H^1 , where $\rho_g(\mathbf{x})$ is a nonnegative minimizer of the energy

$$E_{\delta_\infty}(\sqrt{\rho}) = \int_{\mathbb{R}^d} \left(V(\mathbf{x})\rho - \frac{1}{2}\rho^2 + \frac{\delta_\infty}{2} |\nabla \rho|^2 \right) d\mathbf{x}, \quad \|\rho(\mathbf{x})\|_{L^1} = 1, \quad \rho(\mathbf{x}) \geq 0. \quad (3.25)$$

(2) If $\beta \rightarrow -\infty$ and $\delta/|\beta|^{\frac{4+d}{2+d}} \gg 1$, i.e. $\beta = o(\delta^{\frac{2+d}{4+d}})$ as $\delta \rightarrow +\infty$, set $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \phi_g(\mathbf{x}/\varepsilon) \in S$ with $\varepsilon = \delta^{-\frac{1}{4+d}}$. For $\delta \rightarrow +\infty$ ($\varepsilon \rightarrow 0^+$), we have $\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2$ converges to $\rho_\infty(\mathbf{x})$ in H^1 , where $\phi_\infty(\mathbf{x}) = \sqrt{\rho_\infty(\mathbf{x})}$ is the unique nonnegative minimizer of the energy $E_3(\cdot)$ in (3.6).

(3) If $\beta \rightarrow -\infty$ and $\delta = o(|\beta|^{\frac{4+d}{2+d}})$, we also assume that $V(\mathbf{x})$ is radially symmetric and the ground state $\phi_g \in S$ can be chosen as a decreasing radially symmetric function. Let $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2} \phi_g(\mathbf{x}/\varepsilon) \in S$ with $\varepsilon = |\beta|^{1/2}/\delta^{1/2}$, and $\rho_g^\varepsilon = |\phi_g^\varepsilon|^2 \rightarrow \rho_\infty$ in H^1 as $\beta \rightarrow -\infty$, where ρ_∞ is the unique non-increasing radially symmetric minimizer of the following energy

$$E_r(\sqrt{\rho}) = \int_{\mathbb{R}^d} \left(\frac{1}{2} |\nabla \rho|^2 - \frac{1}{2} |\rho|^2 \right) d\mathbf{x}, \quad \int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} = 1, \quad \rho(\mathbf{x}) \geq 0. \quad (3.26)$$

In fact, ρ_∞ solves the equation

$$-\Delta \rho_\infty - \rho_\infty = \mu \chi_{\{\rho_\infty > 0\}}, \quad \mu = 2E_r(\sqrt{\rho_\infty}). \quad (3.27)$$

Proof (1) The existence of the nonnegative minimizer of E_{δ_∞} can be proved similarly to Theorem 2.1 and we omit the details here for brevity.

Let $\varepsilon = |\beta|^{-\frac{1}{2+d}}$ and $\rho_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d} |\phi_g(\mathbf{x}/\varepsilon)|^2$ where $\phi_g(\mathbf{x})$ is a ground state of (2.1), then $\sqrt{\rho_g^\varepsilon} \in S$ is a ground state of (3.3). Using Nash inequality with the fact $\sqrt{\rho_g^\varepsilon} \in S$, we can easily find

$$\int_{\mathbb{R}^d} V(\mathbf{x}) \rho_g^\varepsilon(\mathbf{x}) d\mathbf{x} + \|\nabla \rho_g^\varepsilon\| + \|\rho_g^\varepsilon\| \leq C. \quad (3.28)$$

We can extract a subsequence $\varepsilon_n \rightarrow 0$, such that for some $\rho_0 \in H^1$, we have

$$\rho_g^{\varepsilon_n} \rightarrow \rho_0, \quad \text{weakly in } H^1, \quad \text{weakly-} \star \quad \text{in } L_V^1 = \{\rho \mid \int_{\mathbb{R}^d} V(\mathbf{x}) |\rho| dx < +\infty\}, \quad (3.29)$$

and

$$\int_{\mathbb{R}^d} V(\mathbf{x}) \rho_0(\mathbf{x}) d\mathbf{x} + \|\nabla \rho_0\| + \|\rho_0\| \leq \liminf_{\varepsilon_n \rightarrow 0^+} \left(\int_{\mathbb{R}^d} V(\mathbf{x}) \rho_g^{\varepsilon_n}(\mathbf{x}) d\mathbf{x} + \|\nabla \rho_g^{\varepsilon_n}\| + \|\rho_g^{\varepsilon_n}\| \right).$$

We then show that the convergence is strong in L^2 . For any $\eta > 0$, there exists $R > 0$ such that $\int_{|\mathbf{x}| > R} \rho_g^{\varepsilon_n}(\mathbf{x}) d\mathbf{x} < \eta$ (confining property of $V(\mathbf{x})$). Since $H^1(B_R) \hookrightarrow L^2(B_R)$ is compact, $\int_{|\mathbf{x}| \leq R} |\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^2 d\mathbf{x} \rightarrow 0$ and

$$\begin{aligned} & \limsup_{\varepsilon_n \rightarrow 0} \|\rho_g^{\varepsilon_n} - \rho_0\|^2 \\ &= \limsup_{\varepsilon_n \rightarrow 0} \int_{|\mathbf{x}| \leq R} |\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^2 d\mathbf{x} + \limsup_{\varepsilon_n \rightarrow 0} \int_{|\mathbf{x}| > R} |\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^2 d\mathbf{x} \\ &\leq \limsup_{\varepsilon_n \rightarrow 0} \left(\int_{|\mathbf{x}| > R} |\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})| d\mathbf{x} \right)^{\frac{1}{2}} \left(\int_{|\mathbf{x}| > R} |\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^3 d\mathbf{x} \right)^{\frac{1}{2}} \\ &\leq C\eta^{1/2}. \end{aligned}$$

Hence $\limsup_{\varepsilon_n \rightarrow 0} \|\rho_g^{\varepsilon_n} - \rho_0\|^2 = 0$ and $\rho_g^{\varepsilon_n} \rightarrow \rho_0$ in L^2 , which implies that $\rho_0(\mathbf{x}) \geq 0$. Similarly, due to the confining property of $V(\mathbf{x})$, $\|\rho_0\|_{L^1} = 1$. In particular, regularizing the minimizers of $E_{\delta_\infty}(\cdot)$ in (3.25) if necessary, we have

$$E_{\delta_\infty}(\sqrt{\rho_0}) \leq \liminf_{\varepsilon^n \rightarrow 0} E_{\delta_\infty}(\sqrt{\rho_g^{\varepsilon^n}}) \leq \limsup_{\varepsilon^n \rightarrow 0} E^{\varepsilon_n}(\sqrt{\rho_g^{\varepsilon^n}}) \leq E^{\varepsilon_n}(\sqrt{\rho_0}),$$

and $E^{\varepsilon_n}(\sqrt{\rho_0}) \leq E_{\delta_\infty}(\sqrt{\rho_0}) + o(1)$, which verifies ρ_0 is a minimizer of $E_{\delta_\infty}(\cdot)$ in (3.25) as well as $\|\nabla \rho_g^{\varepsilon_n}\| \rightarrow \|\nabla \rho_0\|$. Thus, $\rho_g^{\varepsilon_n} \rightarrow \rho_0$ in H^1 .

(2) The proof is similar to part (1) in view of the fact that the minimizer of (3.6) is unique, thus it is omitted here for brevity.

(3) We first show the fact that the decreasing radially symmetric minimizer ρ_∞ of (3.26) exists and is unique. In view of Nash inequality, $E_r(\sqrt{\rho})$ is bounded from below under constraint $\|\rho\|_{L^1} = 1$ with $\rho \geq 0$. By Schwarz rearrangement, we can take a minimizing sequence of nonincreasing radially symmetric functions $\{\rho_n\}_{n=1}^\infty$ where $\|\rho_n\|_{L^1} = 1$ and $\|\rho_n\|_{H^1} \leq C$. Therefore, there exists $\rho_\infty \in H^1$ such that a subsequence (denoted as the original sequence) $\rho_n \rightarrow \rho_\infty$ weakly in H^1 . Applying necessary scaling $\rho_n^\eta = \eta^{-d} \rho_n(\mathbf{x}/\eta)$

($\eta > 0$) in $E_r(\cdot)$, then $E_r(\sqrt{\rho_n^\eta})$ attains its minimum at some $\eta_n > 0$ and we can take $\rho_n^{\eta_n}$ as the minimizing sequence. As a consequence, we can assume $\eta_n = 1$ and have the relation $\|\rho_n\|^2 = \frac{d}{2+d}\|\nabla \rho_n\|^2$ and $E_r(\sqrt{\rho_n}) < 0$ by the optimality of $\eta_n = 1$ among all the possible scalings. In addition, for the nonincreasing radially symmetric function ρ_n ,

$$|\rho_n(\mathbf{x})| \leq \frac{C}{R^d} \|\rho_n\|_{L^1} \leq \frac{C}{R^d}, \quad |\mathbf{x}| \geq R > 0, \quad (3.30)$$

which would imply $\rho_n \rightarrow \rho_\infty$ strongly in L^2 and so $\rho_\infty \geq 0$. In fact, we can show $\|\rho_\infty\|_{L^1} = 1$. Denote $I_\alpha = \inf_{\rho \geq 0, \|\rho\|_{L^1} = \alpha} E_r(\sqrt{\rho})$ ($\alpha > 0$), then it is obvious $I_\alpha = \alpha^2 I_1$ and $I_1 < 0$. If $\|\rho_\infty\|_{L^1} = \alpha < 1$, by the convergence of ρ_n , we get

$$\alpha^2 I_1 = I_\alpha \leq E_r(\sqrt{\rho_\infty}) \leq \liminf_{n \rightarrow +\infty} E_r(\sqrt{\rho_n}) = I_1, \quad (3.31)$$

which leads to $I_1 \geq 0$ contradicting to the fact $I_1 < 0$. Thus $\|\rho_\infty\|_{L^1} = 1$ and ρ_∞ is a non-increasing radially symmetric minimizer of (3.26). Next, we show such a minimizer is unique. Following Theorem 3.2, we can get the equation for the minimizer of (3.26) as

$$-\Delta \rho - \rho = \mu \chi_{\{\rho > 0\}}, \quad (3.32)$$

and a non-increasing radially symmetric minimizer ρ is compactly supported with the regularity stated in Theorem 3.2. If there are two non-increasing radially symmetric minimizers ρ_1 and ρ_2 to the energy (3.26), we have

$$-\Delta \rho_1 - \rho_1 = \mu_1 \chi_{\{\rho_1 > 0\}}, \quad -\Delta \rho_2 - \rho_2 = \mu_2 \chi_{\{\rho_2 > 0\}},$$

and $\mu_1 = \mu_2 = 2I_1$. Thus, by integrating the equations, we know ρ_1 and ρ_2 have the same supports (denote as the ball B_R). $\rho_1 = \rho_2$ is then a consequence of classical ODE theory by noticing that $\rho_j(R) = \partial_r \rho_j(R) = 0$. The existence and uniqueness of non-increasing radially symmetric minimizers are proved.

Next, choosing $\varepsilon = \frac{|\beta|^{1/2}}{\delta^{1/2}}$ in (3.3), we find ϕ_g^ε minimizes the following energy

$$E_\eta(\phi) = \int_{\mathbb{R}^d} \left[\frac{\eta_1}{2} |\nabla \phi|^2 + \eta_2 V(\mathbf{x}) |\phi|^2 - \frac{1}{2} |\phi|^4 + \frac{1}{2} |\nabla |\phi|^2|^2 \right] d\mathbf{x}, \quad \phi \in S, \quad (3.33)$$

with $\eta_1 = \frac{\delta^{\frac{d-2}{2}}}{|\beta|^{\frac{d}{2}}} = o(1)$ and $\eta_2 = \frac{\delta^{\frac{d+2}{2}}}{|\beta|^{\frac{4+d}{2}}} = o(1)$ when $\beta \rightarrow -\infty$ and $\delta = o(|\beta|^{\frac{4+d}{2+d}})$. Intuitively, only the leading $O(1)$ terms in (3.33) are important in the limit as $\beta \rightarrow -\infty$. Under the hypothesis of a radially symmetric increasing potential $V(\mathbf{x})$, we have (regularize $\phi_\infty = \sqrt{\rho_\infty}$ such that $\phi_\infty \in H^1$ if necessary)

$$E_r(\sqrt{\rho_\infty}) \leq E_r(\sqrt{\rho_g^\varepsilon}) \leq E_\eta(\phi_g^\varepsilon) \leq E_\eta(\sqrt{\rho_\infty}) \leq o(1) + E_r(\sqrt{\rho_\infty}), \quad (3.34)$$

which shows $\lim_{\beta \rightarrow -\infty} E_r(\sqrt{\rho_g^\varepsilon}) = E_r(\sqrt{\rho_\infty}) = I_1$. Repeating the previous arguments, we will have $\rho_g^\varepsilon \rightarrow \rho_\infty$ in H^1 . \square

Next, we consider the effects of $\delta \rightarrow 0^+$, i.e. the vanishing higher order effects. It is worth noticing that the ground state profiles will have certain blow-up phenomenon as $\delta \rightarrow 0^+$ in the classical regimes where the ground state does not exist when $\delta = 0$.

Theorem 3.4 (*Limits when $\delta \rightarrow 0^+$*) Let $V(\mathbf{x})$ ($\mathbf{x} \in \mathbb{R}^d$, $d = 1, 2, 3$) be given in (1.8), $\delta > 0$, $\phi_g^\delta \in S$ be a nonnegative ground state of (2.1).

(1) Suppose $\beta > 0$ when $d = 3$, $\beta > -C_b$ when $d = 2$, and $\beta \in \mathbb{R}$ when $d = 1$, where C_b is given in (2.6). There exists a subsequence $\delta_n \rightarrow 0$ ($n = 1, 2, \dots$), such that $\phi_g^{\delta_n}(\mathbf{x}) \rightarrow \phi_g(\mathbf{x})$ in H^1 , where $\phi_g(\mathbf{x})$ is a nonnegative minimizer of the energy

$$E_{\text{GP}}(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi|^2 + V(\mathbf{x}) |\phi|^2 + \frac{\beta}{2} |\phi|^4 \right] d\mathbf{x} \quad \text{with} \quad \|\phi\| = 1. \quad (3.35)$$

Moreover, when $\beta \geq 0$, the nonnegative minimizer ϕ_g of (3.35) is unique and $\phi_g^\delta \rightarrow \phi_g$ in H^1 as $\delta \rightarrow 0^+$.

(2) When $d = 2$ and $\beta < -C_b$, denote $\tilde{\phi}_\delta(\mathbf{x}) = \sqrt{\delta} \phi_g^\delta(\sqrt{\delta} \mathbf{x})$ and we have for a subsequence $\delta_n \rightarrow 0$, $\tilde{\phi}_{\delta_n}(\mathbf{x}) \rightarrow \phi_0(\mathbf{x})$ in H^1 , where $\phi_0(\mathbf{x})$ is a nonnegative minimizer of the energy

$$E_\beta(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi|^2 + \frac{\beta}{2} |\phi|^4 + \frac{1}{2} |\nabla |\phi|^2|^2 \right] d\mathbf{x} \quad \text{with} \quad \|\phi\| = 1. \quad (3.36)$$

(3) When $d = 3$ and $\beta < 0$, we also assume that $V(\mathbf{x})$ is radially symmetric and it is sufficient to consider the ground state $\phi_g^\delta(\mathbf{x})$ as decreasing radially symmetric functions. Let $\tilde{\rho}_\delta(\mathbf{x}) = |\tilde{\phi}_\delta(\mathbf{x})|^2$, where $\tilde{\phi}_\delta(\mathbf{x}) = \delta^{3/4} \phi_g^\delta(\sqrt{\delta} \mathbf{x})$. There exists $0 \leq \rho_0(\mathbf{x}) \in H^1$ such that $\tilde{\rho}_\delta \rightarrow \rho_0$ in H^1 as $\delta \rightarrow 0$, where ρ_0 is the unique decreasing radially symmetric nonnegative minimizer of the energy

$$E_r^\beta(\sqrt{\rho}) = \int_{\mathbb{R}^d} \left[\frac{\beta}{2} |\rho|^2 + \frac{1}{2} |\nabla \rho|^2 \right] d\mathbf{x}, \quad \rho \geq 0, \quad \int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} = 1. \quad (3.37)$$

More precisely, $\rho_0 \geq 0$ satisfies the free boundary problem

$$\beta \rho - \Delta \rho = \mu \chi_{\{\rho > 0\}}, \quad \rho|_{\partial\{\rho > 0\}} = |\nabla \rho|_{\partial\{\rho > 0\}} = 0, \quad (3.38)$$

where $\mu = 2E_r^\beta(\sqrt{\rho_0})$.

Proof (1) The proof is similar to that presented in Theorem 3.3 and is omitted here for brevity.

(2) The existence of the nonnegative minimizer of $E_\beta(\cdot)$ can be proved by a similar argument in Theorem 3.3 for the energy $E_r(\cdot)$ and the detail is omitted here. We denote the minimum energy of $E_\beta(\cdot)$ as E_0 .

Letting $\varepsilon = \delta^{-1/2}$ in (3.3), it is obvious that $\tilde{\phi}_\delta(\mathbf{x}) \in S$ minimizes the energy

$$\tilde{E}_\delta(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi|^2 + \delta^2 V(\mathbf{x}) |\phi|^2 + \frac{\beta}{2} |\phi|^4 + \frac{1}{2} |\nabla |\phi|^2|^2 \right] d\mathbf{x}, \quad \phi \in S. \quad (3.39)$$

Now, choosing a ground state $\phi_g \in S$ of (3.36) as a testing state (using a C_0^∞ approximation if necessary for the potential term), we have

$$\delta^2 \int_{\mathbb{R}^d} V(\mathbf{x}) |\tilde{\phi}_\delta(\mathbf{x})|^2 d\mathbf{x} + E_\beta(\tilde{\phi}_\delta) = \tilde{E}_\delta(\tilde{\phi}_\delta) \leq \tilde{E}_\delta(\phi_g) \leq E_0 + C\delta^2,$$

which implies $\int_{\mathbb{R}^d} V(\mathbf{x}) |\tilde{\phi}_\delta(\mathbf{x})|^2 d\mathbf{x} \leq C$. Therefore, we have

$$\int_{\mathbb{R}^d} V(\mathbf{x}) |\tilde{\phi}_\delta(\mathbf{x})|^2 d\mathbf{x} + \|\tilde{\phi}_\delta\|_{H^1} + \|\nabla |\tilde{\phi}_\delta|^2\| \leq C.$$

Following the proof in Theorem 2.1, there exists $\phi_0 \in H^1$ with $\|\phi_0\| = 1$ and a subsequence $\delta_n \rightarrow 0$ such that $\phi_{\delta_n} \rightarrow \phi_0$ strongly in L^2 and weakly in H^1 ,

$$E_\beta(\phi_0) \leq \liminf_{n \rightarrow \infty} E_\beta(\phi_{\delta_n}) \leq \liminf_{n \rightarrow \infty} \tilde{E}_\delta(\phi_{\delta_n}) \leq E_0,$$

and ϕ_0 is a minimizer of (3.36). From the above inequality, it is easy to find that $\phi_{\delta_n} \rightarrow \phi_0$ strongly in H^1 .

(3) The proof is essentially presented in part (3) of Theorem 3.3. \square

3.2 Box potential case

Now we consider (1.7) defined on a bounded domain $\Omega \subset \mathbb{R}^d$, the limiting profiles of the ground states (2.1) are considered under different sets of parameters δ and β . To simplify the discussion, we choose the external potential as the box potential, i.e.

$$V(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in \Omega, \\ +\infty, & \text{otherwise.} \end{cases} \quad (3.40)$$

The energy $E(\cdot)$ in (1.10) reduces to

$$E_\Omega(\phi) = \int_\Omega \left[\frac{1}{2} |\nabla \phi|^2 + \frac{\beta}{2} |\phi|^4 + \frac{\delta}{2} |\nabla |\phi|^2|^2 \right] d\mathbf{x}, \quad (3.41)$$

and the ground state ϕ_g is then the minimizer of the energy $E_\Omega(\phi)$ under the constraint $\|\phi\|_{L^2(\Omega)} = 1$. The characterization of the ground state ϕ_g for (3.41) in some limiting cases is listed in the following theorems. The major difference between the whole space case (section 3.2) and the bounded domain case is that the scalings are very different.

Theorem 3.5 (*Thomas-Fermi limit*) *Let $V(\mathbf{x})$ be the box potential (3.40), $\delta > 0$, and $\phi_g \in S$ be the positive ground state of (2.1).*

(1) *If $\beta \rightarrow +\infty$ and $\delta = o(\beta)$, we have $\rho_g^\beta = |\phi_g(\mathbf{x})|^2$ converge to $\rho_\infty(\mathbf{x}) := |\phi_\infty(\mathbf{x})|^2$ in L^2 , where $\phi_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy*

$$E_b(\phi) = \int_\Omega \frac{1}{2} |\phi|^4 d\mathbf{x} \quad \text{with} \quad \|\phi\| = 1. \quad (3.42)$$

More precisely, $\rho_\infty = \frac{1}{|\Omega|}$ with $\mu = \frac{\beta}{2|\Omega|}$, where $|\Omega|$ is the volume of the domain Ω .

(2) If $\beta \rightarrow +\infty$ and $\lim_{\beta \rightarrow +\infty} \frac{\delta}{\beta} = \delta_0 > 0$ for some $\delta_0 > 0$, we have $\rho_g^{\beta, \delta} = |\phi_g(\mathbf{x})|^2$ converge to $\rho_\infty(\mathbf{x})$ in H^1 , where $\rho_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy

$$E_{\text{bd}}^+(\sqrt{\rho}) = \int_{\Omega} \left[\frac{1}{2} |\rho|^2 + \frac{\delta_0}{2} |\nabla \rho|^2 \right] d\mathbf{x}, \quad \rho \geq 0, \quad \int_{\Omega} \rho(\mathbf{x}) d\mathbf{x} = 1. \quad (3.43)$$

More precisely, $\rho_\infty(\mathbf{x}) \geq 0$ satisfies the equation

$$\rho_\infty(\mathbf{x}) - \delta_0 \Delta \rho_\infty(\mathbf{x}) = \mu, \quad \mathbf{x} \in \Omega, \quad \rho_\infty(\mathbf{x})|_{\partial\Omega} = 0, \quad (3.44)$$

where $\mu = 2E_{\text{bd}}^+(\sqrt{\rho_\infty})$.

(3) If $\delta \rightarrow +\infty$ and $\beta = o(\delta)$, we have $\rho_g^\delta = |\phi_g(\mathbf{x})|^2$ converge to $\rho_\infty(\mathbf{x})$ in H^1 , where $\rho_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy

$$E_d(\sqrt{\rho}) = \int_{\Omega} \frac{1}{2} |\nabla \rho|^2 d\mathbf{x}, \quad \rho \geq 0, \quad \int_{\Omega} \rho(\mathbf{x}) d\mathbf{x} = 1. \quad (3.45)$$

More precisely, $\rho_\infty(\mathbf{x}) \geq 0$ satisfies the equation

$$-\Delta \rho_\infty(\mathbf{x}) = \mu, \quad \mathbf{x} \in \Omega, \quad \rho_\infty(\mathbf{x})|_{\partial\Omega} = 0, \quad (3.46)$$

where $\mu = 2E_d(\sqrt{\rho_\infty})$.

Proof The proof is similar to those in Theorem 3.1 for the whole space case.

Remark 3.1 In Theorem 3.5, case (3) holds true in the case $\beta \rightarrow -\infty$ and $\delta \gg |\beta|$, i.e. $\beta = o(\delta)$. For case (2), when $\beta \rightarrow -\infty$ and $\lim_{\beta \rightarrow -\infty} \frac{\delta}{|\beta|} = \delta_0 > 0$ for some $\delta_0 > 0$, we have that there exists a subsequence of $\beta_n \rightarrow -\infty$ and δ_n , such that $\rho_g^{\beta_n, \delta_n} = |\phi_g^{\beta_n, \delta_n}(\mathbf{x})|^2$ converges to $\rho_\infty(\mathbf{x})$ in H^1 , and $\rho_\infty(\mathbf{x})$ is a nonnegative minimizer of the energy

$$E_{\text{bd}}^-(\sqrt{\rho}) = \int_{\Omega} \left[-\frac{1}{2} |\rho|^2 + \frac{\delta_0}{2} |\nabla \rho|^2 \right] d\mathbf{x}, \quad \rho \geq 0, \quad \int_{\Omega} \rho(\mathbf{x}) d\mathbf{x} = 1. \quad (3.47)$$

It remains to consider the last case in Theorem 3.5 as $\beta \rightarrow -\infty$ and $\delta = o(|\beta|)$. For simplicity, we assume Ω is a ball in \mathbb{R}^d .

Theorem 3.6 Let $\Omega = B_R = \{|\mathbf{x}| < R\}$ in the box potential given in (3.40), $\beta < 0$ and $\delta > 0$, $\phi_g^\beta \in H^1(\Omega)$ be a non-increasing radially symmetric ground state of (3.41). Define $\tilde{\phi}_g^\beta \in H^1(\mathbb{R}^d)$ such that $\tilde{\phi}_g^\beta(\mathbf{x}) = 0$ when $\mathbf{x} \notin \Omega$, and $\tilde{\phi}_g^\beta(\mathbf{x}) = \phi_g^\beta(\mathbf{x})$ when $\mathbf{x} \in \Omega$. Let $\tilde{\phi}_g^\varepsilon(\mathbf{x}) = \varepsilon^{d/2} \tilde{\phi}_g^\beta(\mathbf{x}\varepsilon) \in S$ with $\varepsilon = \delta^{1/2}/|\beta|^{1/2}$, thus $\varepsilon \rightarrow 0^+$ as $\beta \rightarrow -\infty$. We have $\tilde{\rho}_g^\varepsilon = |\tilde{\phi}_g^\varepsilon|^2 \rightarrow \rho_\infty$ in H^1 as $\varepsilon \rightarrow 0^+$, where ρ_∞ is the unique non-increasing radially symmetric minimizer of energy $E_r(\cdot)$ in (3.26).

Proof Let $\Omega^\varepsilon = \{\mathbf{x}/\varepsilon, \mathbf{x} \in \Omega\}$. Since ρ_∞ is compactly supported as shown in Theorem 3.3, for sufficiently small $\varepsilon > 0$, we have $\text{supp}(\rho_\infty) \subset \Omega^\varepsilon$. On the other hand, ϕ_g^ε minimizes the energy

$$E_{\text{box}}^\eta(\phi) = \int_{\mathbb{R}^d} \left[\frac{\eta}{2} |\nabla \phi|^2 - \frac{1}{2} |\phi|^4 + \frac{1}{2} |\nabla |\phi|^2|^2 \right] d\mathbf{x}, \quad \phi \in H_0^1(\Omega^\varepsilon), \quad \|\phi\| = 1, \quad (3.48)$$

where $\eta = \frac{\delta \frac{d-2}{2}}{|\beta|^{\frac{d}{2}}} = o(1)$ as $\varepsilon \rightarrow 0^+$. We can then proceed as that in Theorem 3.3 and the limit of $\tilde{\rho}^\varepsilon$ as $\beta \rightarrow -\infty$ ($\varepsilon \rightarrow 0^+$) follows. \square

Similarly, we could extend the $\delta \rightarrow 0^+$ limiting results in Theorem 3.4 to the bounded domain case too. Since no different scaling is involved, the extension is straightforward and we omit it here for brevity.

4 Dynamics of the MGPE

In this section, we investigate the dynamics of BEC with HOI governed by the MGPE (1.7). In particular, we would like to see how the δ term affects the dynamics. It is worth pointing out that the local well-posedness of the MGPE (1.7) with the initial data

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad (4.1)$$

has been established [32, 29]. Accordingly, we will assume the MGPE (1.7) admits a smooth solution $\psi(\mathbf{x}, t)$ in the subsequent discussion.

4.1 Dynamical properties

As mentioned before, the MGPE (1.7) conserves the energy (1.10) and the mass (L^2 -norm) (1.9). In this part, we will show the behavior of some other important quantities, namely the momentum, the center of mass and angular momentum expectation, that measure the dynamical properties of BEC with HOI.

Consider the momentum defined as

$$\mathbf{P}(t) = \int_{\mathbb{R}^d} \text{Im}(\bar{\psi}(\mathbf{x}, t) \nabla \psi(\mathbf{x}, t)) d\mathbf{x}, \quad t \geq 0, \quad (4.2)$$

where $\text{Im}(f)$ and \bar{f} denote the imaginary part and complex conjugate of f , respectively. Then we have the following result.

Lemma 4.1 *Assume $\psi(\mathbf{x}, t)$ is a sufficiently smooth solution of (1.7) with (4.1) and $|\nabla V(\mathbf{x})| \leq C(V(\mathbf{x}) + 1)$ for $\mathbf{x} \in \mathbb{R}^d$, then we have*

$$\dot{\mathbf{P}}(t) = - \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 \nabla V(\mathbf{x}) d\mathbf{x}, \quad t \geq 0. \quad (4.3)$$

In particular, the momentum is conserved if $V(\mathbf{x}) \equiv C_0$ with C_0 a constant.

Proof The proof is a generalization of the one shown in [9,6]. To be more specific, differentiating (4.2) with respect to t , recalling (1.7) and integrating by parts, we have

$$\begin{aligned}\dot{\mathbf{P}}(t) &= -i \int_{\mathbb{R}^d} [\bar{\psi}_t \nabla \psi - \psi_t \nabla \bar{\psi}] d\mathbf{x} = \int_{\mathbb{R}^d} [(-i\bar{\psi}_t) \nabla \psi + i\psi_t \nabla \bar{\psi}] d\mathbf{x} \\ &= \int_{\mathbb{R}^d} \left[\left(-\frac{1}{2} \nabla^2 \bar{\psi} + V(\mathbf{x}) \bar{\psi} + \beta |\psi|^2 \bar{\psi} - \delta \nabla^2 |\psi|^2 \bar{\psi} \right) \nabla \psi + c.c. \right] d\mathbf{x},\end{aligned}$$

where $c.c.$ denotes the complex conjugate of the first part in the integral. A simple computation implies that

$$\int_{\mathbb{R}^d} [-\delta \nabla^2 |\psi|^2 \bar{\psi} \nabla \psi - \delta \nabla^2 |\psi|^2 \psi \nabla \bar{\psi}] d\mathbf{x} = \frac{\delta}{2} \int_{\mathbb{R}^d} \nabla (|\nabla |\psi|^2|^2) d\mathbf{x} = 0,$$

while the integral of the remaining terms is shown in [9,6] to be

$$\int_{\mathbb{R}^d} \left[\left(-\frac{1}{2} \nabla^2 \bar{\psi} + V(\mathbf{x}) \bar{\psi} + \beta |\psi|^2 \bar{\psi} \right) \nabla \psi + c.c. \right] d\mathbf{x} = - \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 \nabla V(\mathbf{x}) d\mathbf{x},$$

and thus we complete the proof. \square

The center of mass is another important quantity to describe the dynamics and is defined as

$$\mathbf{x}_c(t) = \int_{\mathbb{R}^d} \mathbf{x} |\psi(\mathbf{x}, t)|^2 d\mathbf{x}, \quad t \geq 0, \quad (4.4)$$

and we can get the following lemma describing the motion of \mathbf{x}_c ,

Lemma 4.2 *Assume $\psi(\mathbf{x}, t)$ is a sufficiently smooth solution of (1.7) with (4.1), then we have*

$$\dot{\mathbf{x}}_c(t) = \frac{i}{2} \int_{\mathbb{R}^d} [\psi \nabla \bar{\psi} - \bar{\psi} \nabla \psi] d\mathbf{x}, \quad \ddot{\mathbf{x}}_c(t) = - \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 \nabla V(\mathbf{x}) d\mathbf{x}. \quad (4.5)$$

Proof Analogous to the calculation in Lemma 4.1, we get

$$\dot{\mathbf{x}}_c(t) = \frac{i}{2} \int_{\mathbb{R}^d} [\psi \nabla \bar{\psi} - \bar{\psi} \nabla \psi] d\mathbf{x} = \mathbf{P}(t), \quad t \geq 0,$$

and then $\ddot{\mathbf{x}}_c(t)$ follows the result in Lemma 4.1.

In 2D and 3D cases, we also consider the angular momentum expectation defined as

$$\langle L_z \rangle = \int_{\mathbb{R}^d} \bar{\psi} L_z \psi d\mathbf{x} = i \int_{\mathbb{R}^d} \bar{\psi} (y \partial_x - x \partial_y) \psi d\mathbf{x}, \quad (4.6)$$

and we have the following lemma on the dynamical law of the angular momentum expectation with a harmonic potential.

Lemma 4.3 Assume $\psi(\mathbf{x}, t)$ is a sufficiently smooth solution of (1.7) with (4.1) and $d \geq 2$ and $V(\mathbf{x})$ is a harmonic potential (1.8), then we have

$$\frac{d\langle L_z \rangle}{dt} = \int_{\mathbb{R}^d} (\gamma_x^2 - \gamma_y^2) xy |\psi(\mathbf{x}, t)|^2 d\mathbf{x}, \quad t \geq 0. \quad (4.7)$$

Consequently, the angular momentum expectation is conserved if $\gamma_x = \gamma_y$.

Proof The proof is a generalization of the proof for $\delta = 0$ case shown in [9, 6, 8]. For simplicity, we consider the case $d = 2$. The case $d = 3$ can be derived in a similar way. Differentiate $\langle L_z \rangle$ with respect to t , we get

$$\begin{aligned} \frac{d\langle L_z \rangle}{dt} &= i \int_{\mathbb{R}^d} [\bar{\psi}_t (y \partial_x - x \partial_y) \psi + \bar{\psi} (y \partial_x - x \partial_y) \psi_t] d\mathbf{x} \\ &= \int_{\mathbb{R}^d} \left[\left(-\frac{1}{2} \nabla^2 \bar{\psi} + V(\mathbf{x}) \bar{\psi} + \beta |\psi|^2 \bar{\psi} - \delta \nabla^2 |\psi|^2 \bar{\psi} \right) (x \partial_y \psi - y \partial_x \psi) + c.c. \right] d\mathbf{x}. \end{aligned}$$

From results in [9, 6, 8], for the part without δ , we have

$$\begin{aligned} &\int_{\mathbb{R}^d} \left[\left(-\frac{1}{2} \nabla^2 \bar{\psi} + V(\mathbf{x}) \bar{\psi} + \beta |\psi|^2 \bar{\psi} \right) (x \partial_y \psi - y \partial_x \psi) + c.c. \right] d\mathbf{x} \\ &= \int_{\mathbb{R}^d} (\gamma_x^2 - \gamma_y^2) xy |\psi|^2 d\mathbf{x}. \end{aligned}$$

For the remaining term, i.e. terms containing δ , we have

$$\begin{aligned} &\int_{\mathbb{R}^d} [-\delta \nabla^2 |\psi|^2 \bar{\psi} (x \partial_y \psi - y \partial_x \psi) - \delta \nabla^2 |\psi|^2 \psi (x \partial_y \bar{\psi} - y \partial_x \bar{\psi})] d\mathbf{x} \\ &= \delta \int_{\mathbb{R}^d} \nabla |\psi|^2 \cdot \nabla (x \partial_y |\psi|^2 - y \partial_x |\psi|^2) d\mathbf{x} \\ &= \delta \int_{\mathbb{R}^d} \left[\frac{1}{2} \partial_y (x |\nabla |\psi|^2|^2) - \frac{1}{2} \partial_x (y |\nabla |\psi|^2|^2) + \nabla |\psi|^2 \cdot \begin{pmatrix} \partial_y |\psi|^2 \\ -\partial_x |\psi|^2 \end{pmatrix} \right] d\mathbf{x} \\ &= 0. \end{aligned}$$

The conclusion follows directly from the above results. \square

Comparing with $\delta = 0$ case [9, 6], we find the δ term does not affect the dynamical laws of momentum, center-of-mass and the angular momentum expectation in an explicit way.

4.2 An analytical solution of the MGPE

In this section, we construct an exact solution of the MGPE (1.7) with the external potential to be the harmonic potential (1.8) and the initial data to be a stationary state with its center-of-mass shifted. This kind of analytical solution is useful in practice, especially for the validation of numerical schemes.

To be more specific, let $\phi_s(\mathbf{x})$ be a stationary state of the MGPE (1.7) with chemical potential μ_s , i.e.

$$\mu_s \phi_s(\mathbf{x}) = -\frac{1}{2} \nabla^2 \phi_s + V(\mathbf{x}) \phi_s + \beta |\phi_s|^2 \phi_s - \delta \nabla^2 |\phi_s|^2 \phi_s, \quad \|\phi_s\| = 1. \quad (4.8)$$

Then we have the following lemma.

Lemma 4.4 *Suppose $V(\mathbf{x})$ is given by (1.8) and the initial data (4.1) is chosen as*

$$\psi_0(\mathbf{x}) = \phi_s(\mathbf{x} - \mathbf{x}_0) e^{i(\mathbf{k}_0 \cdot \mathbf{x} + \omega_0)}, \quad \mathbf{x} \in \mathbb{R}^d, \quad (4.9)$$

where $\mathbf{x}_0 \in \mathbb{R}^d$, $\mathbf{k}_0 \in \mathbb{R}^d$ and $\omega_0 \in \mathbb{R}$ are given. Then the solution of (1.7) with (4.9) can be expressed as

$$\psi(\mathbf{x}, t) = \phi_s(\mathbf{x} - \mathbf{x}_c(t)) e^{-i\mu_s t} e^{i(\mathbf{k}(t) \cdot \mathbf{x} + \omega(t))}, \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0, \quad (4.10)$$

where $\mathbf{x}_c(t)$ satisfies the second order ODE

$$\ddot{\mathbf{x}}_c(t) + A \mathbf{x}_c(t) = 0, \quad t > 0, \quad (4.11)$$

with the initial data

$$\mathbf{x}_c(0) = \mathbf{x}_0, \quad \dot{\mathbf{x}}_c(0) = \mathbf{k}_0, \quad (4.12)$$

and A is a $d \times d$ matrix defined as $A = (\gamma_x^2)$ when $d = 1$, $A = \text{diag}(\gamma_x^2, \gamma_y^2)$ when $d = 2$ and $A = \text{diag}(\gamma_x^2, \gamma_y^2, \gamma_z^2)$ when $d = 3$. The equations governing $\mathbf{k}(t)$ and $\omega(t)$ can also be derived as

$$\dot{\mathbf{k}}(t) = -A \mathbf{x}_c(t), \quad \dot{\omega}(t) = -\frac{|\mathbf{k}|^2}{2} - \frac{1}{2} \mathbf{x}_c^T A \mathbf{x}_c, \quad t > 0, \quad (4.13)$$

respectively, with the initial data

$$\mathbf{k}(0) = \mathbf{k}_0, \quad \omega(0) = \omega_0. \quad (4.14)$$

Proof An analogous reasoning for $\delta = 0$ case in [9, 6, 8] is applied here. Differentiating (4.10) with respect to t and \mathbf{x} respectively, plugging in the MGPE (1.7), changing the variable $\mathbf{x} - \mathbf{x}_c(t) \rightarrow \mathbf{x}$, and using the fact that ϕ_s is a stationary state, we get

$$\begin{aligned} & -i \partial_t \mathbf{x}_c \cdot \nabla \phi_s(\mathbf{x}) - (\partial_t \mathbf{k} \cdot \mathbf{x} + \partial_t \omega(t)) \phi_s(\mathbf{x}) \\ & = -i \mathbf{k} \cdot \nabla \phi_s(\mathbf{x}) + \frac{|\mathbf{k}|^2}{2} \phi_s + (V(\mathbf{x} + \mathbf{x}_c) - V(\mathbf{x})) \phi_s(\mathbf{x}). \end{aligned}$$

We can see that the δ term does not introduce new terms in this procedure compared to the conventional GPE, i.e. $\delta = 0$ case [9, 6, 8]. As a result, we will get the same result. The details are omitted here for brevity. \square

4.3 Finite time blow-up

By the local well-posedness [32, 29], we expect a local smooth solution of the MGPE (1.7) for smooth initial data. Below, we show a criteria when a smooth solution of (1.7) develops finite time singularity. We will need the following lemma on the time evolution of the variance defined as

$$\delta_\alpha(t) = \int_{\mathbb{R}^d} \alpha^2 |\psi(\mathbf{x}, t)|^2 d\mathbf{x}, \quad t \geq 0, \quad (4.15)$$

with α being either x , y or z . We have the following lemma regarding the dynamic of the quantity.

Lemma 4.5 *Assume $\psi(\mathbf{x}, t)$ is a sufficiently smooth solution of (1.7) with (4.1), and denote $\rho = |\psi|^2$, then we have*

$$\dot{\delta}_\alpha(t) = i \int_{\mathbb{R}^d} \alpha (\psi \partial_\alpha \bar{\psi} - \bar{\psi} \partial_\alpha \psi) d\mathbf{x}, \quad t \geq 0, \quad (4.16)$$

$$\ddot{\delta}_\alpha(t) = \int_{\mathbb{R}^d} [2|\partial_\alpha \psi|^2 + (\beta\rho - 2\alpha \partial_\alpha V(\mathbf{x}))\rho + 2\delta|\partial_\alpha \rho|^2 + \delta|\nabla \rho|^2] d\mathbf{x}. \quad (4.17)$$

Proof Differentiating (4.15) with respect to t , applying (1.7) and integrating by parts, we get (4.16). (4.17) can be obtained similarly.

Theorem 4.1 *Assume $V(\mathbf{x})$ is smooth and satisfies $V(\mathbf{x})d + \mathbf{x} \cdot \nabla V(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^d$. For any smooth solution $\psi(\mathbf{x}, t)$ of the MGPE (1.7) with (4.1), if $\int_{\mathbb{R}^d} |\mathbf{x}|^2 |\psi_0|^2 d\mathbf{x} < \infty$, $\delta < 0$ and $d = 2, 3$, there exists finite time blow-up if one of the following holds:*

- (i) $E(\psi_0) < 0$,
- (ii) $E(\psi_0) = 0$ and $i \int_{\mathbb{R}^d} [\mathbf{x} \cdot (\psi_0 \nabla \bar{\psi}_0 - \bar{\psi}_0 \nabla \psi_0)] d\mathbf{x} < 0$,
- (iii) $E(\psi_0) > 0$ and $i \int_{\mathbb{R}^d} [\mathbf{x} \cdot (\psi_0 \nabla \bar{\psi}_0 - \bar{\psi}_0 \nabla \psi_0)] d\mathbf{x} < -2\sqrt{E(\psi_0)d} \|\mathbf{x}\psi_0\|_2$.

Proof Lemma 4.5 shows that for the variance $\delta_\mathbf{x}(t) = \int_{\mathbb{R}^d} |\mathbf{x}|^2 |\psi(\mathbf{x}, t)|^2 d\mathbf{x}$, $\dot{\delta}_\mathbf{x}(t) = i \int_{\mathbb{R}^d} [\mathbf{x} \cdot (\psi \nabla \bar{\psi} - \bar{\psi} \nabla \psi)] d\mathbf{x}$ and

$$\begin{aligned} \ddot{\delta}_\mathbf{x}(t) &= \int_{\mathbb{R}^d} [2|\nabla \psi|^2 - 2|\psi|^2 \mathbf{x} \cdot \nabla V(\mathbf{x}) + \beta|\psi|^4 d + (d+2)\delta|\nabla|\psi|^2|^2] d\mathbf{x} \\ &= 2E(\psi)d - (d-2)\|\nabla \psi\|^2 + 2\delta\|\nabla|\psi|^2\|^2 - 2 \int_{\mathbb{R}^d} |\psi|^2 (\mathbf{x} \cdot \nabla V(\mathbf{x}) + V(\mathbf{x})d) d\mathbf{x} \\ &< 2E(\psi_0)d, \quad t > 0. \end{aligned}$$

Therefore, we get

$$\delta_\mathbf{x}(t) \leq E(\psi_0)t^2 d + \dot{\delta}_\mathbf{x}(0)t + \delta_\mathbf{x}(0), \quad t \geq 0. \quad (4.18)$$

There exists a finite time $0 < T < +\infty$ such that $\delta_\mathbf{x}(T) < 0$ if one of (i), (ii) and (iii) is satisfied. It means there exists a singularity at or before $t = T$. \square

It is interesting to see that for $\delta < 0$, there exists smooth ψ_0 such that $E(\psi_0) < 0$ even if $\beta > 0$, while the MGPE (1.7) with $\beta > 0$ and $\delta = 0$ is globally well-posed [6]. As a consequence, a HOI term with $\delta < 0$ will cause the dynamical instability of the underlying BEC system.

We note that the local well-posedness of the MGPE (1.7) in the energy space is not available yet. The above results are based on the assumption that $\psi(\mathbf{x}, t)$ is a smooth solution of the MGPE (1.7) with (4.1).

5 Conclusion

We have analyzed the ground states and dynamics of a Bose-Einstein condensate (BEC) in the presence of higher-order interactions (HOI), modelled by a modified Gross-Pitaevskii equation (MGPE). The ground state structures are quite different from the case without HOI. We established the existence and uniqueness as well as non-existence results on ground states in different parameter regimes. The asymptotic profiles of the ground states under different combinations of HOI and contact interaction strengths were studied. The limiting profiles were found to be quite interesting and complicated involving free boundary problems. Finally, some discussions on the dynamics of BEC with HOI were carried out.

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